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Investigation of cetane number and octane number correlation under homogenous-charge compression-ignition engine operation

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Abstract

A novel fuel-substitution strategy was used to investigate the relationship between octane number and cetane number under representative low temperature combustion (LTC) thermodynamic conditions. The cetane number of the test fuels was known by using mixtures of the cetane number secondary reference fuels (SRFs) T-26 and U-19, which are full-blend certification fuels used in the place of 2,2,4,4,6,8,8-heptamethylnonane and *n*-hexadecane for engine cetane number testing. The octane number was derived from the fuel-substitution methodology in terms of the octane primary reference fuel (PRF, consisting of *n*-heptane and isooctane) mixture needed to maintain combustion phasing during homogeneous-charge compression-ignition (HCCI) engine operation as increasing amounts of the SRF mixture was substituted for the PRF mixture. A linear blending relationship was found to exist between the cetane and octane numbers. Results agree with other similar relationships from the literature acquired under substantially different operating conditions. The current study significantly expands the range of the cetane–octane correlation to a range of cetane numbers from 20 to 75 and validates the correlation at low equivalence ratios of interest to LTC operation.

Keywords: Cetane; Octane; SRF; LTC

1. Introduction

Octane and cetane ratings are two important parameters that describe a fuel's ignition qualities. The octane number is related to the fuel's resistance to autoignition and is an important indicator of engine knock, which ultimately limits a spark-ignition engine's compression ratio and, thus, efficiency. The cetane number describes a fuel's propensity to ignite, and plays a vital role for compression ignition (CI) engines.

The octane number (ON) of a fuel is experimentally found using both the research octane number (RON) and motored octane number (MON) methods as specified by ASTM D2699 and D2700, respectively [1,2]. The octane number determined by either test refers to the mixture of octane number primary reference fuels (PRFs)

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isooctane (2,2,4-trimethylpentane) and *n*-heptane that exhibits a standardized knocking intensity at the same compression ratio (CR) as the test fuel for prescribed operating conditions. The resulting octane number corresponds to the volumetric percentage of isooctane in the PRF mixture. The RON test conditions are: intake air temperature of 52 °C and ambient pressure, spark ignition timing 13° before top dead center (bTDC), and an engine speed of 600 rpm. The MON test conditions are: intake air temperature of 149 °C and ambient pressure, spark ignition timing of 26° to 14° bTDC depending on engine CR, and an engine speed of 900 rpm. Both tests use a variable CR engine (ranging from 4 to 18), and fuels typically tested using these methods have octane ratings between 40 and 100. Due to the low speeds and high intake temperatures used in these tests, numerous studies have found that fuel reactivity cannot be adequately described by the RON and MON tests; many fuels exhibit a strong sensitivity to engine operating conditions [9,10]. Therefore, it is useful to have the ability to test fuels of interest at a variety of different engine-relevant operating conditions; the current testing method will be described in more detail later in the paper.

Cetane number (CN) is found using a variable CR pre-chamber diesel engine according to ASTM D613 [3]. The cetane number of a fuel, refers to the mixture of cetane number primary reference fuels isocetane (2,2,4,4,6,8,8-heptamethylnonane) and n-hexadecane that exhibits the same ignition delay of 13 crank angle degrees (CAD) at the same CR for a set engine operating condition. The cetane test conditions specify an intake air temperature of 66 °C and ambient pressure with a start of injection (SOI) occurring in the pre-chamber at 13° before top dead center. Compression ratio, which can vary between 8 and 36, is adjusted until ignition occurs at TDC. Typical diesel fuels tested have cetane numbers between 30 and 65. In practice, due to the high cost of the cetane primary reference fuels, secondary reference fuels (SRFs) T and U, which are tightly controlled full-blend fuels made by Chevron Phillips, are used for testing. The specific SRFs used in this study are T-26 and U-19, having tested cetane numbers of 75.2 and 19.4, respectively.

Formerly, a direct comparison between gasoline-like fuels described by octane number and diesel-like fuels specified described by cetane number was not necessary since they had separate applications; high-octane (low reactivity) fuels were predominantly used in SI engines while high-cetane (high reactivity) fuels were used in CI engines. However, due to the increased interest in LTC, combustion strategies are being investigated involving the compression-ignition of low-reactivity fuels [4], and the use of mixtures of low- and high-reactivity fuels in dual-fuel combustion strategies [5]. Many of these strategies utilize fully or partially premixed quantities of fuel at much lower than stoichiometric equivalence ratios. An advantage of using a HCCI testing method is that it allows for the ignition quality of the fuel to be characterized fully by its kinetic behavior while avoiding fuel spray injection complications.

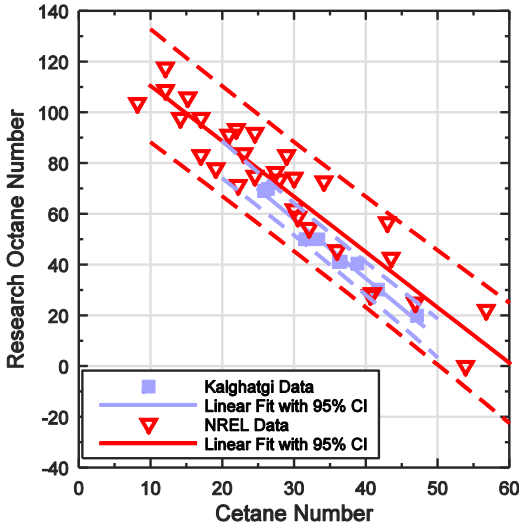

Fig. 1. Cetane number as a function of RON. Data compiled from [6] and [7].

Computational fluid dynamics (CFD) is an important tool for the investigation and development of low temperature combustion strategies. However, the implementation of detailed chemistry of large molecules, like those found in diesel fuel, in CFD is still beyond the capability of current computing power for engineering applications. Thus, simplified chemistry needs to be used. The most common surrogate for diesel fuel in CFD is *n*-heptane because skeletal chemical kinetics models are available. Skeletal models also exist for the PRF blends. A well-established link between cetane number and octane number would potentially allow more accurate CFD modeling of fuels, *i.e.*, it would provide an easy-to-implement means for varying the cetane number.

Direct comparisons of the cetane and octane number have been undertaken using the results of RON/MON and cetane testing. Kalghatgi [6] measured the cetane number of PRF blends and mixtures of *n*-heptane and toluene, and compared them to their measured (or known) research octane numbers (RON). The results showed a linear correlation between the two metrics. The National Renewable Energy Laboratory (NREL) [7] compiled results for an array of single-component hydrocarbons, including oxygenates, and also recovered a linear relation between RON and cetane number. These results are reproduced in Fig. 1, including confidence intervals that arise from the linear fitting. The results in tabular form can be found in