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Ignition studies of two low-octane gasolines

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ABSTRACT

Low-octane gasolines (RON ~ 50–70 range) are prospective fuels for gasoline compression ignition (GCI) internal combustion engines. GCI technology utilizing low-octane fuels has the potential to significantly improve well-to-wheel efficiency and reduce the transportation sector's environmental footprint by offsetting diesel fuel usage in compression ignition engines. In this study, ignition delay times of two low-octane FACE (Fuels for Advanced Combustion Engines) gasolines, FACE I and FACE J, were measured in a shock tube and a rapid compression machine over a broad range of engine-relevant conditions (650–1200 K, 20 and 40 bar and $\phi = 0.5$ and 1). The two gasolines are of similar octane ratings with anti-knock index, AKI = (RON + MON)/2, of ~ 70 and sensitivity, S = RON–MON, of ~ 3. However, the molecular compositions of the two gasolines are notably different. Experimental ignition delay time results showed that the two gasolines exhibited similar reactivity over a wide range of test conditions. Furthermore, ignition delay times of a primary reference fuel (PRF) surrogate (n-heptane/iso-octane blend), having the same AKI as the FACE gasolines, captured the ignition behavior of these gasolines with some minor discrepancies at low temperatures ($T < 700$ K). Multi-component surrogates, formulated by matching the octane ratings and compositions of the two gasolines, emulated the autoignition behavior of gasolines from high to low temperatures. Homogeneous charge compression ignition (HCCI) engine simulations were used to show that the PRF and multi-component surrogates exhibited similar combustion phasing over a wide range of engine operating conditions.

1. Introduction

The transportation sector accounts for around half of global oil consumption and about 23% of global CO_2 emissions [1,2]. At the 2015 United Nations Climate Change Conference (COP 21, Paris), 196 countries reached an agreement to implement stringent emission regulations and work on strategies that would limit the environmental impact of global warming. The improvements in the transportation sector are necessary to reduce its environmental footprint from the perspective of CO_2 emissions as well as harmful NO_X/unburnt HC/soot emissions. Due to the higher efficiencies of compression ignition engines, several strategies are being explored to use gasoline-like fuels in these engines. Variants of these engine technologies include gasoline compression ignition (GCI), dual-fuel reactivity controlled compression ignition (RCCI), and partially premixed compression ignition (PPCI). These modes of engine operation offer wide ranging potential to increase engine efficiency while reducing harmful environmental emissions compared to traditional compression ignition engines [3].

Gasoline compression ignition (GCI) engines have several advantages over conventional spark ignition gasoline and compression ignition diesel engines. These engines operate at higher compression ratios thus improving overall thermal efficiency which makes these engines comparable to the compression ignited diesel engines [4]. Several studies have demonstrated that GCI engines can operate optimally with fuels having octane numbers ranging 50 – 70 [5–7]. Utilization of low-octane gasolines eliminates refinery catalytic reforming and isomerization units required for the production of high-octane gasolines. This may significantly reduce the refinery costs and subsequent emissions from refinery processing as compared to the conventional gasolines with higher octane rating. Life cycle analysis [1] of GCI engines employing low-octane fuels predicts about 25% reduction in energy consumption and about 23% reduction in CO_2 emissions compared to the conventional spark ignition engines and gasolines. Moreover, there is growing disparity between the demand of diesel and gasoline

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Table 1
Properties of FACE gasolines I and J, multi-component and PRF surrogates. Hydrocarbon types are given in mole %.

	FACE I	FGI-KAUST surrogate	FACE J	FGJ-KAUST surrogate	PRF 70 surrogate
RON	70.3	70.7	71.8	70.6	70
MON	69.6	68.4	68.8	66.5	70
Sensitivity	0.7	2.3	3	4.1	0
AKI	69.9	69.6	70.3	68.6	70
Avg. mol. wt.	95.5	98.9	100.2	103.2	109.7
n-alkanes	14	12	31.5	35	33
iso-alkanes	70	72	32.4	35	67
Cycloalkanes	4	6	2.4	–	0
Aromatics	5	4	30.6	30	0
Olefins	7	6	0.6	–	0
Unidentified	–	–	2.5	–	–

fuels resulting in lighter fractions of hydrocarbons being in oversupply [8]. Such imbalance can also be potentially solved by employing GCI engine technologies that operate with lighter hydrocarbon streams and can thereby reduce the operational challenges faced by many refineries around the world.

Combustion phasing in GCI engines are largely governed by chemical kinetics [9]. However, combustion chemistry of low-octane gasolines is relatively less studied as compared to conventional gasolines. The only previous contributions to the chemical kinetics of fully blended low-octane gasolines are from our group at KAUST [10–13]. Javed et al. [10] studied the ignition delay times and surrogate formulation of light naphtha, a low-octane (RON = 64.5, MON = 63.5) fully blended fuel, in a high-pressure shock tube and rapid compression machine over wide range of test conditions. They showed that at high temperatures and in the negative temperature coefficient (NTC) region, a primary reference fuel (PRF) surrogate (mixture of n-heptane and iso-octane) adequately captured the autoignition of light naphtha; while at low temperatures, a multi-component surrogate better reproduced the ignition behavior of light naphtha. Javed et al. [11] and Abbad et al. [12] provided a wide range of ignition delay data for toluene/PRF (TPRF) and PRF blends with research octane numbers (RON) ranging 70–97.5 to model the reactivity of low-to-high octane gasolines.

At the Clean Combustion Research Center (CCRC) of King Abdullah University of Science and Technology (KAUST), significant efforts have been devoted towards formulating surrogates and developing combustion kinetics of gasolines with varying compositions and octane numbers [10,14–18]. Sarathy et al. [14] studied the ignition delay times of FACE (Fuels for Advanced Combustion Engines) gasolines A and C using shock tubes and rapid compression machines, and developed multi-component surrogates for these gasolines based on detailed hydrocarbon analyses (DHA). The FACE gasolines A and C had similar octane numbers (AKI ~ 84) but contained varying amounts of n-alkanes, iso-alkanes and aromatics. It was shown that these two gasolines exhibited comparable ignition delay times at all experimental conditions and a PRF surrogate adequately captured the ignition requirements of these gasolines with minor discrepancies at low temperatures. Sarathy et al. [15] also studied the ignition behavior and surrogate formulation of FACE gasolines F and (RON = 94.4, MON = 88.8) and G (RON = 96.8, MON = 85.8) having similar antiknock indices (AKI ~ 91.5) but varying octane sensitivities and compositions. They showed that at high temperatures ($T > 900$ K), ignition delay times of both gasolines were quite similar. However, at low temperatures ($T < 750$ K), gasoline with lower RON (FACE F) was slightly more reactive compared to the high-RON gasoline (FACE G), and the fuel with low sensitivity (FACE F) showed greater NTC behavior. Finally, gasoline with lower MON (FACE G) was more reactive in 800–900 K temperature range. Based on DHA analysis, multi-component surrogates were developed for FACE F and G and it was shown that multi-component surrogate simulations better captured the ignition behavior of high sensitivity gasolines.

The current study aims to continue our efforts of formulating surrogates for wide variety of gasolines and improving the chemical kinetic modeling of these fuels. Specific objectives of the current study are two-fold; first, we aim to provide new ignition delay data for two low-octane FACE gasolines (FACE I and J); second, we wish to provide adequate surrogate formulation guidelines for such low-octane fuels. As mentioned earlier, ignition delay data are scarce for low-octane gasolines, and, hence, the data reported herein serves as valuable benchmark for future studies. The manuscript is structured as follows: fuel characterization using DHA analysis, gasoline properties and the tested surrogates are presented in Section 2, experimental techniques are briefly presented in Section 3, ignition delay results are presented and discussed in Section 4, chemical kinetic analyses are presented in Section 5 to illustrate the reactivity trends, HCCI engine simulations are included in Section 6 to assess how different surrogates affect combustion phasing, and the key findings of this work are summarized in Section 7.

2. Fuel characterization and surrogate formulation of FACE gasolines I and J

The two fully blended gasoline fuels studied in this work, FACE gasoline I and J, were acquired from Conoco Phillips Chemical Company. Fuel compositions and other relevant properties are listed in Table 1 (See also Supplementary material Tables S1–S2 for Detailed Hydrocarbon Analysis, Figs. S1–S2 for a comparison between PIONA and ADC of fuels and surrogates). FACE I is highly paraffinic (~ 84 mol %) and has low aromatic (~ 5 mol %) and olefinic (~ 7 mol %) content. FACE J has relatively less paraffinic content (~ 64 mol %) but it contains larger fraction of aromatics (~ 30 mol %). FACE gasolines I and J have relatively low octane sensitivities of 0.7 and 3, respectively. The two fuels, with widely different compositions, have very similar anti-knock index ($AKI = \frac{RON+MON}{2}$) of ~ 70.

Gasoline reactivity is compared against two kinds of surrogates. A binary PRF surrogate, mixture of n-heptane/iso-octane, matching the AKI of the FACE I and J is used as the simplest surrogate. Multi-component surrogate mixtures formulated for FACE I