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Manifestation of octane rating, fuel sensitivity, and composition effects for gasoline surrogates under advanced compression ignition conditions

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ABSTRACT

Substantial research effort has been spent on the development of advanced compression ignition (ACI) engine combustion strategies over the past decades, including homogeneous charge compression ignition (HCCI), reactivity controlled compression ignition (RCCI), and gasoline direct-injection compression-ignition (GDCI), etc. The behavior of gasoline-type fuels under compression ignition conditions has subsequently attracted extensive experimental and kinetic modeling interest. On the other hand, towards the development of future transportation fuels and engines, the evaluation of general fuel properties, instead of endless testing of specific fuels, should be the future research focus. In this study, the individual roles of the research and motor octane numbers (i.e., RON and MON) and fuel sensitivity (S) in characterizing the ignition performance of gasoline surrogates have been systematically investigated under a typical ACI engine condition using well-validated surrogate and kinetic models. The crank angle corresponding to 50% total heat release (CA50) was utilized as an indicator of the overall fuel reactivity, and iso-contours of CA50 were mapped out in the full engine operating domain characterized by the temperature and pressure at intake valve closing (IVC). By comparing the ignition performance of toluene primary reference fuel blends (TPRF) with the same RON, MON or S values, the distinctive effects and dominant ACI operating conditions of these fuel properties are clearly demonstrated. The role of equivalence ratio is also discussed by comparing the intrinsic stoichiometric condition of the standard octane rating tests and the lean mixture conditions required by ACI operation. The results show that octane sensitivity manifests itself in the high pressure low temperature operating regime for fuels with identical RON or MON, through different low temperature reactivities and heat release rates, while in low pressure high temperature conditions, combustion phasing is less sensitive to all fuel properties, including RON, MON and S. TPRFs with the same sensitivity show the largest variation of CA50 in the intermediate operating conditions, where the thermodynamic traces pass primarily through the ignition delay regime characterized by negative-temperature coefficient (NTC) behavior. Finally, by comparing the combustion phasing of five different gasoline surrogates with nearly identical RON and MON, potential compositional effects for gasoline fuels under ACI condition are further discussed via kinetic modeling. This study also demonstrates that the controlling fuel properties of gasoline-like fuels depend on ACI operating conditions (pressure and temperature trajectory), which should be carefully considered when constructing fuel metrics and comparing experimental results of ACI engines.

1. Introduction

For decades, gasoline fuels have attracted extensive research interest for its applications in both traditional naturally aspirated and modern boosted downsized spark-ignition (SI) engines. Due to its multi-component nature, different surrogate models have been developed to model gasoline and its engine combustion performance, such as primary reference fuels (PRF), which are blends of n-heptane and iso-octane [1], toluene primary reference fuel blends (TPRF) with the addition of toluene [2] representing aromatic components and contributing octane sensitivity, and several more detailed surrogates which include more chemical components and classes [3–6]. Among these surrogates, TPRF models are frequently

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used due to their simplicity and ability to simultaneously match the base fuel's research octane number (RON) and motor octane number (MON) [2]. Meanwhile, many chemical kinetic models [6–9] have been further developed to describe the combustion chemistry of TPRF blends, with satisfactory performance in reproducing fundamental combustion targets including laminar flame speed, speciation during homogeneous oxidation, and autoignition delay time, etc. A thorough overview of different surrogate models and kinetic mechanisms for gasoline is seen recently in [10].

Due to the major advantages of diesel-like efficiency and the ability of operating in the low-temperature combustion (LTC) regime characterized by both low NO_x and soot formation, advanced compression ignition (ACI) combustion strategies have attracted extensive research effort in the recent developments of internal combustion engines. These strategies include homogeneous charge compression ignition (HCCI) [11,12], premixed charge compression ignition (PCCI) [13,14], and reactivity controlled compression ignition (RCCI) [15,16], etc. These novel combustion strategies largely rely on the compression ignition of homogeneous or moderately stratified fuel/air mixtures under highly-boosted, dilute intake conditions to operate in the LTC regime, such that the corresponding combustion phasing is dominated by fuel ignition kinetics. Among these advanced engine combustion strategies, gasoline direct injection compression ignition (GDCI) is of particular interest [17–24], where LTC can be achieved by late or multiple injections of gasoline-like fuels with relatively long ignition delay and high volatility during the compression stroke, with high compression ratio. The behavior of gasoline-type fuels under compression ignition conditions has subsequently attracted extensive research interest.

With distinct combustion strategies and operating conditions compared to conventional spark-ignition (SI) engines, metrics for comprehensive fuel reactivity and sensitivity in ACI engines are urgently needed to provide direct guidance on fuel screening and engine optimization in the development of future ACI engines and potential fuels. In the recent Co-Optima program of the US Department of Energy, this point has been made clear with the central hypothesis that if general fuel properties could be suitably characterized by a merit function, then two fuels with the same merit values are expected to share the same engine performance under these same operating conditions. The key to this idea is that instead of testing and screening numerous specific fuels individually, a more proper focus should be fuel properties, which are more general and useful. These fuel properties include flame speed, ignition delay, volatility, emission generation and so on, and serve as the basis for fuel merit function construction.

For ignition screening, the simplest course is to assume that fuels properties based on some traditional, readily available metrics such as RON and MON and fuel sensitivity (S = RON–MON) could also work in ACI strategies. Along these lines, the octane index, OI (OI = RON–K*S), where K is a parameter that relates to the operating condition, has been proposed and used to predict fuel ignition performance under the simplest ACI mode – HCCI conditions [25–27]. However, a few studies have shown the drawback of the OI correlation, depending on either engine operating strategy [28,29] or fuel compositions [27,30]. Specifically, Koopmans et al. [29] observed that HCCI engines operated with negative valve overlap (NVO) are much less sensitive to fuel ignitability than those with direct heated intake air. Farrell and Bunting [28] further confirmed such observations and found substantial difference in ignition timing for 6 fuels with the same RON and MON under identical HCCI engine operating conditions. Consequently, more concerns have been raised on the kinetic effect of the internally trapped hot residual in conjunction with potential fuel composition effects. It is further shown that the original OI correlation is not able to capture the HCCI ignitability for fuels with high ethanol [27,30] or high aromatic content [30]. As such, alternative indexes and methodologies are still being developed and investigated to better correlate combustion phasing in HCCI engines, including the HCCI index [31], Lund-Chevron HCCI Number [32], the modified JKZ OI [30], and staged Livengood–Wu integral [33]. From the kinetic modeling perspective, recent work by Tao et al. [34] studied the role of fuel properties RON, MON and S in the description of general fuel reactivity and sensitivity under typical HCCI conditions, based on well-validated combustion kinetic mechanisms and calculated iso-contours of combustion phasing. One of the major findings in [34] was that even for fuels with the same RON and MON (e.g., n-pentane vs. PRF62), combustion phasing under the same ACI operating conditions can be significantly different.

These studies inspire the current work to further understand the relevance of traditional fuel property metrics, and potential compositional effects in ACI engines for gasoline-like fuels, with well-controlled intake valve closing (IVC) mixture conditions. The rationales from a fundamental perspective are as below. First, the conventional octane rating is a global parameter which largely reflects the competition between flame propagation and auto-ignition during knock in the cooperative fuel research (CFR) engine. Due to the largely similar flame propagation behavior of gasoline fuels (especially for those without high ethanol content) [35], their performance in a purely kinetically-controlled ACI environment may therefore be reasonably correlated with RON and MON. Second, the testing conditions corresponding to RON and MON are both naturally aspirated and do not cover a typical boosted condition with elevated intake pressure. It is hence possible that the limitations on the standard RON/MON test constrain their application as universal criteria for fuel reactivity in ACI conditions. Third, engines equipped with ACI strategies typically operate under lean compression ignition conditions, while the end gas during the CFR engine knocking combustion is largely stoichiometric, which therefore raises concerns regarding equivalence ratio effects. Last, with previous experimental results shedding light on composition effects, it will be intriguing to further look into any potential composition effects for multicomponent gasoline surrogates. Therefore, the investigation targets: (1) understanding how RON, MON and S *individually* manifest themselves in ACI conditions; (2) evaluating equivalence ratio effects on ACI combustion phasing; (3) identifying potential compositional effects on ACI combustion phasing for multicomponent gasoline surrogates.

This work is based upon substantial progresses made in gasoline surrogate modeling and kinetic mechanism development within the past decades. The literature reported surrogate and kinetic models for TPRFs and multicomponent gasoline surrogates are carefully reviewed and evaluated. Overall fuel reactivity is indicated by the combustion phasing CA50 (the crank angle corresponding to 50% of heat release), and iso-contours of CA50 under different IVC conditions, denoted here as inlet conditions, are mapped out from the well-validated kinetic model for a wide range of inlet temperatures and pressures. From the CA50 iso-contours, the sensitivity of the fuel to the inlet conditions can be assessed by the change in CA50 as a function of the variation of operating conditions. The performance of gasoline surrogates with the same RON, MON or S is systematically compared to show the operating conditions over which these parameters influence the combustion phasing, and how each parameter influences the sensitivity of the fuel to operating conditions. While we do not expect direct quantitative agreement with engine combustion experiments, we do believe that the sensitivity of combustion phasing to the variation of fuel properties and engine operating conditions should be qualitatively predicted using these mechanisms. The results thereby provide useful insights on the role of traditional fuel properties, and guidance on the construction of ignition merit functions for gasoline fuels in ACI engines.