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Autoignition of straight-run naphtha: A promising fuel for advanced compression ignition engines

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ABSTRACT

Naphtha, a low-octane distillate fuel, has been proposed as a promising low-cost fuel for advanced compression ignition engine technologies. Experimental and modelling studies have been conducted in this work to assess autoignition characteristics of naphtha for use in advanced engines. Ignition delay times of a certified straight-run naphtha fuel, supplied by Haltermann Solutions, were measured in a shock tube and a rapid comparison machine over wide ranges of experimental conditions (20 and 60 bar, 620–1223 K, $\phi = 0.5$, 1 and 2). The Haltermann straight-run naphtha (HSRN) has research octane number (RON) of 60 and motor octane number (MON) of 58.3, with carbon range spanning C3–C9. Reactivity of HSRN was compared, via experiments and simulations, with three suitably formulated surrogates: a two-component PRF (n-heptane/iso-octane) surrogate, a three-component TPRF (toluene/n-heptane/iso-octane) surrogate, and a six-component surrogate. All surrogates reasonably captured the ignition delays of HSRN at high and intermediate temperatures. However, at low temperatures ($T < 750$ K), the six-component surrogate performed the best in emulating the reactivity of naphtha fuel. Temperature sensitivity and rate of production analyses revealed that the presence of cyclo-alkanes in naphtha inhibits the overall fuel reactivity. Zero-dimensional engine simulations showed that PRF is a good autoignition surrogate for naphtha at high engine loads, however, the six-component surrogate is needed to match the combustion phasing of naphtha at low engine loads.

1. Introduction

The rapid increases in population and living standards in developing countries are expected to increase global demand for transportation energy at an annual rate of 1–1.5% through at least 2050 [1–4]. Despite strong growth in alternative energy, traditional petroleum-based fuels (gasoline, diesel and jet fuel) are expected to dominate the transportation energy portfolio, both for light- and heavy- duty applications [2–4]. In addition, there is ample evidence that sufficient crude reserves exist to meet this increased demand [4,5]. A major concern of the utilization of fossil fuels is the emission of greenhouse gases (GHG) which impose significant burden on our environment. As a result, regulatory authorities are enforcing stringent efficiency and emissions regulations on the transportation sector. Therefore, improving the fuel efficiency in the transportation sector can help reduce the global energy usage and minimize GHG emissions.

Various advanced compression ignition engines have been investigated as technologies that combine the best of gasoline and diesel engines. Combustion strategies such as homogeneous charge compression ignition (HCCI) [6], reactivity-controlled compression ignition (RCCI) [7–9], and partially-premixed compression ignition (PPCI) [10–13] have sought to combine the relatively simple design of gasoline engines and their after treatment systems and the higher efficiencies of diesel engines benefits. These engine technologies share some high-level characteristics even though the engine operating parameters such as timing and number of injections, fuel type, and air system requirements may differ. Compression ignition operation eliminates traditional engine knock observed in spark-ignition (SI) engines, and globally lean operation eliminates throttling losses. At the same time, greater mixing of fuel and air prior to combustion reduces soot production relative to the conventional mixing-controlled (diesel) combustion.

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Table 1
Properties of Haltermann straight naphtha (HSRN) and its surrogates. Detailed compositions of the three surrogates are available in Table S2 (Supplementary materials).

	HSRN	PRF 60	TPRF 60	MCS
RON	60	60	60[a]	60.5[a]
MON	58.3	60	58.3[a]	58.3[a]
Sensitivity (RON – MON)	1.7	0	1.7	2.2
H/C ratio	2.147	2.264	2.175	2.139
Avg. mol. wt.	92.406	108.201	106.465	95.545
n-alkanes (mole%)	36.7	42.9	42.9	38.6
iso-alkanes (mole%)	37.8	57.1	44.9	41.7
Cycloalkanes (mole%)	15	0	0	8.7
Aromatics (mole%)	10.5	0	12.2	11

[a] Calculated values.

The specifications of the enabling fuel for this engine technology are not very obvious. Many fuels with varying physical and chemical properties, such as ignition quality, distillation curve and chemical compositions, have been considered in previous works. These include conventional gasoline [3,14–18], conventional diesel [11,14,17–22], gasoline–diesel blends ("dieseline") [3,21,23–25], low-octane gasolines ("naphthas") [3,10,12,14–16,26] and reference fuel blends (composed of iso-octane, n-heptane, toluene) [3,14,16,27,28]. Certain fuel properties could affect the performance of the engine because PPCI combustion is dependent on mixture stratification as well as chemical kinetics [29] .For example, some studies indicate that there are direct impacts of fuel distillation and aromatic content on the soot emissions of PPCI engines [21,30], while others report a minimal effect [31]. Nonetheless, most of the studies have shown that fuel reactivity, or homogeneous ignition delay, is an important factor in optimizing the performance of PPCI engines over wide range of operating conditions. Optimization of engine in computation fluid dynamic simulations requires the use of simpler surrogate mixtures which mimic the characteristics of real fuel. The surrogates for gasoline-like fuels range from simple binary or ternary mixtures of iso-octane, n-heptane and toluene to more complex mixtures containing additional species such as n-butane, iso-pentane, cyclo-pentane, 1-hexene, 1-pentene, 1,2,4-trimethylbenzene, and others. Many studies are available in literature on surrogate formulation strategies to match the chemical characteristics of real fuels but most previous work was focused on gasoline and diesel [32].

Compared to commercial gasoline and diesel fuels, refinery streams such as petroleum naphtha with research octane numbers (RON) in the 50–80 range have recently been considered attractive alternatives to provide suitable chemical characteristics (longer ignition delay than diesel) in compression ignition engines. These naphtha fuels can be produced in the refinery at lower cost and result in decreased well-to-tank CO_2 emissions. Hao et al. [33] found that compared with the conventional pathway, the low-octane fuel and gasoline compression ignition (GCI) pathway leads to a 24.6% reduction in energy consumption and a 22.8% reduction in GHG emissions.

These low-octane naphtha fuels have not been studied as much as gasoline and diesel fuels. The fundamental characterization of these fuels in terms of homogeneous ignition delay times, laminar flame speeds and speciation is scarce in literature. In fact, the only detailed autoignition study on a real naphtha stream was recently reported by KAUST [32]. Using shock tube and rapid compression machine, Javed et al. [32] measured the homogeneous ignition delay times of a light naphtha stream (RON = 64) along with its primary reference fuel (PRF) and multi-component surrogates over wide ranges of pressures, temperatures and equivalence ratios. They found that the PRF surrogate had similar ignition delay times compared to light naphtha at high and intermediate temperatures. However, a more complex multi-component surrogate was required to match the ignition delay times of light naphtha at low temperatures.

The purpose of the current study is to understand the autoignition behavior of a straight-run naphtha stream with RON of 60 and MON of 58.3. Fuel reactivity is studied using a shock tube and a rapid compression machine at various pressures, temperatures and equivalence ratios which are relevant to the compression ignition engine operation mode. Simple (PRF, TPRF) and more complex (multi-components) surrogates are formulated and their ignition delay times are compared with those of the naphtha fuel. In addition, engine simulations are performed under different engine operating conditions to identify regimes wherein surrogate composition notably alters combustion behavior.

2. Experimental details

2.1. Fuel characterization and surrogate formulation

The naphtha fuel used in this work was purchased from Haltermann Solutions, and is referred as Haltermann straight-run naphtha (HSRN). The certificate of analysis (CoA) and detailed hydrocarbon analysis (DHA) of the fuel are provided in the Supplementary Materials. The fuel primary contains C3–C9 hydrocarbons and does not have any oxygenated species or olefins. The fuel comprises 75% (by mole) paraffinic species and approximately 15% naphthenes and 10% aromatics. The fuel's boiling point range is 32–140 °C and has an average molecular weight of 92.4. The light naphtha studied by Javed et al. [32] primarily consisted of *n*- and *iso*- paraffins, and had higher octane rating than the straight run naphtha used in the current work.

Measured ignition delay times of Haltermann straight-run naphtha (HSRN) are compared with measured and simulated ignition delay times of three surrogates over a range of temperatures, pressures and equivalence ratios. The surrogates are formulated based on the matching of various target properties; (i) a simple two-components surrogate matching the research octane number (RON) of HSRN, (ii) a three-component surrogate matching RON and MON of HSRN, (iii) a six-component surrogates matching RON, MON, H/C, average molecular weight, density, and carbon types.

The two-component PRF surrogate contains 60% iso-octane and 40% n-heptane by volume, and is referred as PRF 60. The three-component TPRF (toluene/n-heptane/iso-octane) surrogate was formulated to match the RON and MON of the naphtha using the methodology proposed by Kalghatgi et al. [34], and is referred as TPRF 60. Studying PRF and TPRF surrogates provide guidance on the conditions (temperatures, pressures and equivalence ratios) under which such simple surrogates may be utilized to mimic the ignition properties of a complex real fuel such as HSRN. This is useful for performing computational fluid dynamic (CFD) simulations, which must use widely available reduced chemical kinetic mechanisms [12,13,35].

The six-component surrogate for HSRN is prepared following the approach presented by Ahmed et al. [36]. This methodology for surrogate fuel formulation involves selection of target properties and carries out an optimization routine on a set of pallet species to achieve the best match with selected target properties. The formulated surrogate consists of n-pentane, n-heptane, 2-methylhexane, 2,2,4-trimethylpentane, cyclopentane and toluene. Basic properties of these species are listed in *Table S1 (Supplementary Materials)*. Octane numbers, RON and MON, of the six-component surrogates were calculated using linear-by-mole correlation, while density was predicted using Refprop [37] at 288 K. The six-component surrogate is referred as MCS (multi-component surrogate) in the remainder of the manuscript.