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Ignition delay measurements of light naphtha: A fully blended low octane fuel

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Abstract

Light naphtha is a fully blended, low-octane (RON = 64.5, MON = 63.5), highly paraffinic (> 90% paraffinic content) fuel, and is one of the first distillates obtained during the crude oil refining process. Light naphtha is an attractive low-cost fuel candidate for advanced low-temperature compression ignition engines where autoignition is the primary control mechanism. We measured ignition delay times for light naphtha in a shock tube and a rapid compression machine (RCM) over a broad range of temperatures (640–1250 K), pressures (20 and 40 bar) and equivalence ratios (0.5, 1 and 2). Ignition delay times were modeled using a two-component primary reference fuel (PRF) surrogate and a multi-component surrogate. Both surrogates adequately captured the measured ignition delay times of light naphtha under shock tube conditions. However, for low-temperature RCM conditions, simulations with the multi-component surrogate showed better agreement with experimental data. These simulated surrogate trends were confirmed by measuring the ignition delay times of the PRF and multi-component surrogates in the RCM at $P = 20$ bar, $\varphi = 2$. Detailed kinetic analyses were undertaken to ascertain the dependence of the surrogates' reactivity on their chemical composition. To the best of our knowledge, this is the first fundamental autoignition study on the reactivity of a low-octane fully blended fuel and the use of a suitably formulated multi-component surrogate to model its behavior.

Keywords: Light naphtha; Low-octane fuel; Ignition delay times; Surrogate formulation; Shock tube

1. Introduction

Petroleum-based liquid fuels, such as gasoline, diesel, jet fuel and heavy oil, currently supply 95%

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of the energy used in the transportation sector [1]. Improving fuel efficiency in this sector can therefore help to reduce global energy usage and minimize greenhouse gas emissions. Advanced low-temperature gasoline (or gasoline/diesel hybrid) engines, homogeneous charge compression ignition (HCCI), dual-fuel reactivity-controlled compression ignition (RCCI), partially premixed compression ignition (PPCI) and other gasoline compression ignition (GCI) variants, in one form or another, are controlled predominantly by chemical kinetics [2]. Correct representation of the fuel ignition kinetics is key if such systems are to be successfully modeled, as autoignition is the primary control mode in these combustion systems. Due to limitations of computational resources, simulations often rely on binary or multi-component fuel surrogates to mimic the behavior of the real fuel.

Petroleum naphtha (also known as hydrobate), with a Research Octane Number (RON) in the 50 – 70 range, has been proposed as a candidate fuel for advanced combustion modes [3–5]. Such low-octane fuels are attractive since they provide sufficient mixing and appropriate chemical propensity due to longer ignition delay times than diesel. Additionally, petroleum naphtha requires much less refinery processing than gasoline, thereby reducing CO_2 emissions from the refining process. The overall result is that the well-to-tank (WTT) greenhouse gas emissions can be minimized [4].

Experimental investigations of petroleum naphtha fuels are scarce [3–8] in the literature and the autoignition characteristics of such fuels have not been studied previously in fundamental combustion experiments. Chang et al. [3,4] studied light and heavy naphtha in PPCI engines and found that the use of petroleum naphtha in PPCI mode can indeed result in overall efficiency improvements and reductions in pollution. Yang et al. [5] showed that hydrobate (RON ~ 69) was less reactive than the corresponding PRF mixture under HCCI conditions. Yang et al. [6,7] utilized double and multiple injection strategies on a single cylinder diesel engine operating with straight-run naphtha fuel (RON ~ 58.8) and showed that multiple injection strategies are advantageous for NOx reduction and efficiency improvements. Detailed experimental and CFD investigations (with surrogate fuels) are needed if petroleum naphtha is to be introduced as a viable future fuel in the transportation sector.

Primary reference fuel (PRF) surrogates (mixtures of *n*-heptane and *iso*-octane), are the simplest and most widely investigated gasoline surrogates. Since a PRF surrogate is composed only of paraffinic fuels, it has zero sensitivity. Sensitivity is defined as the difference between the research (RON) and motor (MON) octane numbers, and is a measure of the non-paraffinic nature of a fuel. Commercial gasolines can have a high content of aromatics (~20 – 30%) and other non-paraffinic (~5 – 10%) species [9], giving the fuel high sensitivity. More complex surrogates are needed to represent the reactivity of high-sensitivity fuels. Typically, toluene is added to PRF mixtures as a substitute for the aromatic compounds present in commercial gasolines. These three-component surrogates are referred to as ternary (or toluene) reference fuels. For a typical ternary surrogate, the toluene concentration is fixed at around 10 – 20% by volume, to achieve an H/C ratio close to that of real gasolines [10], and the PRF composition is then varied to match the octane rating (RON/MON). Gauthier et al. [11] studied the autoignition characteristics of RD387 gasoline and a ternary surrogate (63% *iso*-octane, 20% toluene, 17% *n*-heptane by volume) at high pressures behind reflected shock waves. They showed that the ternary surrogate adequately captured the auto-ignition behavior of a full-blend gasoline at high temperatures ($T > 850$ K). Chaos et al. [10] studied a ternary surrogate in a variable pressure flow reactor and developed an optimized kinetic mechanism. Kukkadapu et al. [12] extended the ignition studies of RD387 gasoline to low temperatures in a rapid compression machine. Kukkadapu et al. [13,14] reported better agreement of a four-component surrogate (*iso*-octane, *n*-heptane, toluene and 2-pentene) with low-temperature ignition delay times for RD387, compared to the ternary surrogate used by Gauthier et al. [11].

More systematic approaches to formulate surrogates based on targeted optimization of palette species yield multi-component (three or more components) surrogates [15–19]. Dooley et al. [15,16], in their works on jet fuel surrogate formulation, have proposed a strategy to emulate the active radical pool formed after initial fuel consumption. Their methodology does not require detailed a priori knowledge of the fuel composition, and the surrogate is formulated by optimizing the average molecular weight (MW), H/C ratio, derived cetane number (DCN), and threshold sooting index (TSI) of those palette species that produce a noticeably different radical pool from each other. Mueller et al. [17] have framed an approach to formulate diesel surrogates based on targeted nonlinear multi-objective optimization of fuel composition, ignition quality, volatility, and density. Ahmed et al. [18] have developed a novel computational architecture that couples CHEMKIN-PRO with an optimization scheme to formulate surrogates that emulate physical and chemical properties of real fuels.

The purpose of this study is to investigate the auto-ignition characteristics of a low-octane fuel and propose a suitable kinetic surrogate. Ignition delay times are measured for Saudi Aramco's light naphtha fuel over a wide range of test conditions using a high pressure shock tube and a rapid compression machine. Measured data are compared against the simulations of a simple PRF surrogate