Surrogate fuel formulation for light naphtha combustion in advanced combustion engines

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Abstract

Crude oil once recovered is further separated in to several distinct fractions to produce a range of energy and chemical products. One of the less processed fractions is light naphtha (LN), hence they are more economical to produce than their gasoline and diesel counterparts. Recent efforts have demonstrated usage of LN as transportation fuel for internal combustion engines with slight modifications. In this study, a multicomponent surrogate fuel has been developed for light naphtha fuel using a multi-variable nonlinear constrained optimization scheme. The surrogate, consisting of palette species *n-pentane, 2-methylhexane, 2-methylbutane, n-heptane* and *toluene,* was validated against the LN using ignition quality tester following ASTM D6890 methodology. Comparison of LN and the surrogate fuel demonstrated satisfactory agreement.

Introduction

A major portion of global industrial and transportation energy demands are met by oil and its derivatives. This trend will continue due to rapid growth and industrialization of developing countries on the Asian and African continents. There is a major thrust of legislation for sustainable energy sources like wind and solar. Nevertheless, oil based products will continue to play an indispensable role for the foreseeable future. One of the primary uses of refined oil products is in automotive transportation. Crude oil is a finite resource, so it must be consumed in the cleanest and most efficient manner.

Once recovered, crude oil is separated into various fractions based on boiling characteristics. One such fraction is light naphtha (LN). LN is one of the least processed streams from the refinery, which makes it relatively inexpensive to produce and environmentally more friendly. Lower emissions with satisfactory combustion efficiency has been observed when LN has been used in IC engines [1] accompanying different combustion strategies. In order to exploit the benefits of lower cost and smaller environmental impact, LN is studied as a potential transportation fuel. Recent efforts [2-6] demonstrated that LN is a viable alternative with advanced combustion strategies like HCCI, PPCI, etc.

In order to realize the maximum potential of LN as a transportation fuel, detailed computational studies concentrating on combustion chemistry are required. This will help in developing a comprehensive understanding of this fuel and its burning characteristics. To enable computational studies, a simple surrogate fuel resembling LN in several physical and chemical properties has to be formulated. After a surrogate fuel is determined and validated, a detailed chemical kinetic model has to be either developed or identified for the surrogate palette species. To arrive at a surrogate fuel, a computational approach has been identified by Ahmed et al. [7]. As per the methodology outlined in [7], the first step is to conduct a Detailed Hydrocarbon Analysis (DHA). For this study, a batch of LN and fuel properties along with DHA (in compliance with standards ASTM D-6733 [8] and ASTM D-6730 [8]) was made available by Saudi Aramco. DHA identified ~ 98 vol % of species present in the fuel. The LN was found to be primarily comprised of 55 vol % of C5-C6 paraffins, 37 vol % of C6-C7 iso-paraffins, 5 vol % of C5 naphthenes and 1 vol % of C6 aromatics.

Proceeding with surrogate fuel formulation, palette species were identified in line with DHA as *n-pentane, 2-methylhexane, 2-methylbutane, n-heptane* and *toluene*. Each molecule has been selected as a representative of a hydrocarbon class. A surrogate is meant to represent the real fuel in terms of certain matching physical and chemical properties, termed target properties. The target properties identified for this study are:

- Hydrogen to carbon ratio
- Density
- Carbon Types[9]
- Research Octane Number
- Volatility Characteristics
- Molecular weight

The DHA is categorized into 11 different carbon types[9] mole fractions following the scheme presented in Figure 1.

Present work focuses on advancing the efforts to develop light naphtha stream as a transportation fuel for advanced combustion engines. This study takes course of developing and validating surrogate fuel for LN to evolve and enhance computational simulation studies across various combustors.

Carbon Type Classification of C to C bonds

1. *n*-CH₃ - primary carbon
2. *n*-CH₂ - secondary carbon
3. *iso*-CH - tertiary carbon
4. *cyclo-alkane* - CH₂ - secondary carbon
5. *cyclo-alkane to alkyl* - tertiary carbon
6. *cyclo-alkane to cyclo-alkane*-tertiary carbon
7. *aromatic* CH - tertiary carbon
8. *aromatic to alkyl* C-quaternary carbon
9. *aromatic to cyclo-alkane* C-quaternary carbon
10. *aromatic to aromatic* C - quaternary carbon
11. *aliphatic* C - quaternary carbon

Figure 1: Carbon Type classification scheme employed in present study

A surrogate fuel has to undergo rigorous experimental validations before it could be established as a reliable model of real fuel. Autoignition characteristics is one of such critical aspects in which surrogate fuel has to emulate real fuel characteristics. In this study autoignition experiments are conducted with LN and LN_surr in ignition quality tester (preheated and pressurized constant volume chamber) to study their autoignition behavior. This study characterizes spray effects and also quantifies the ignition delay.

Surrogate Fuel Formulation

The surrogate fuel formulation scheme specified in [7] has been modified for this study to incorporate a different RON correlation described in Ghosh et al. [10]. After identifying the surrogate palette and target properties, a multi-variable nonlinear constrained optimization outlined in [7] is implemented to arrive at a suitable surrogate composition matching Light Naphtha in all its target properties.

The surrogate is referred as LN_surr and its composition is presented in Table 1:

Table 1: Composition of surrogate LN_surr in Mol %

CAS #	Species	Mol %
78-78-4	2-Methylbutane	0.21
591-76-4	2-Methylhexane	0.07
109-66-0	n-Pentane	0.6
142-82-5	n-Heptane	0.07
108-88-3	Toluene	0.05

Density, H/C ratio and RON are important fuel properties governing several practical aspects of combustion in IC

engines, as well as other applications. For instance, density governs the flow of fuel mass flow rate into combustion chamber. H/C dictates the energy density and has a strong influence on laminar and turbulent burning velocities of fuels. RON determines the tendency to avoid knock when fuel is exposed to higher compression ratios in engines. A comparison of Density, H/C ratio, RON, and Molecular weight between fuel and proposed surrogate fuel is presented in Table 2.

Table 2: Comparison of properties: LN and LN_surr

Properties	LN	LN_surr
Density (Kg/m3 @ 293 k)	642	645
H/C	2.32	2.31
RON	64.5	64.75
Molecular Wt.	78.31	77.92

Volatility is an important aspect of fuel characterization as it dictates the evaporation of fuel in high temperature conditions. It is an important fuel property whether the application is premixed combustion as in Gasoline engine or diffusion driven combustion in Diesel engine. An advanced distillation curve [11] (ADC) has been calculated for the surrogate fuel using Refprop [12] to address volatility characteristics. Due to limited access to the necessary experimental apparatus for measurement of ADC, for this study, the ASTM-D86 [8] measurement has been approximated as ADC for LN. Figure 2 represents the comparison of volatility aspects of LN and LN_surr.
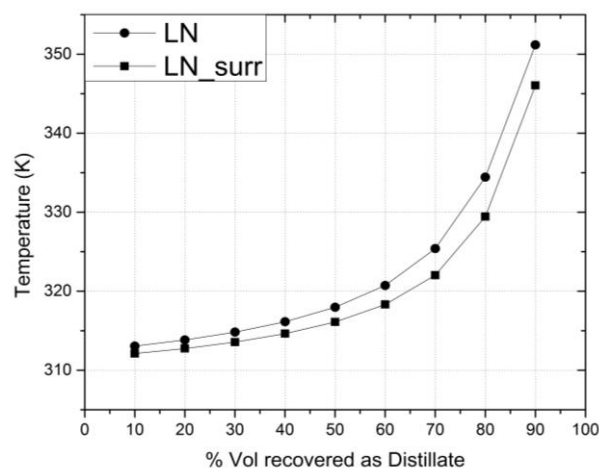
Figure 2: Comparison of distillation curves for Light Naphtha (ASTM D-86) and its surrogate (ADC)

Carbon type classification of the DHA can help capture the reactivity of the hydrocarbon mixture. The reactivity of individual fuel components depends on the types carbon atoms, H abstraction sites, and stability of radicals. Hence it becomes important for a surrogate fuel to match real fuel in carbon types to emulate similar reactivity.

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The quantification of carbon type mole fraction follows the correlation described in [7]. In Figure 3, a comparison is presented between carbon type mole fractions of Light Naphtha fuel and its surrogate. A satisfactory agreement is observed.
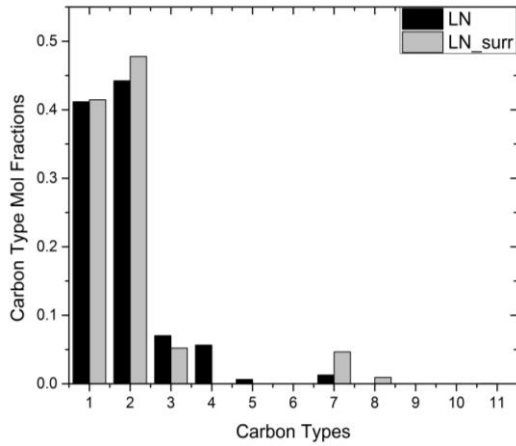

Figure 3: Carbon type comparisons for Light Naphtha and LN_surr

LN_surr is found to match LN in all target properties closely. Hence LN_surr could be studied further for experimental validation. Such surrogates with several physical and chemical properties similar to the real fuel would enable CFD studies for simulating internal combustion engines. Such computational studies provide a wide scope of improvement from fuel injection to combustion till pollutant formations.

Ignition Quality Tester

The KR-IQT (Kaust Research IQT) is a bench-scale constant volume combustion chamber test device to measure ignition delay (ID)/derived cetane number (DCN) of liquid fuels in compliance with ASTM D6890[8]. The KR-IQT makes use of a liquid fuel spray injection system to inject fuel into a pressurized oxidizing environment (air in this case). The fuel injector has a single-hole S-type pintle nozzle. The fuel is delivered to the injector with a mechanical pump driven pneumatically with air at a pressure of 1.2 MPa. The fuel injector sprays liquid fuel at constant pressure of 18 MPa for all test conditions. The scheme is presented in Figure 4.
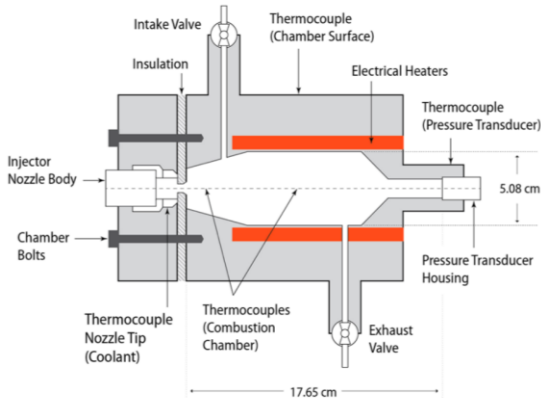

Figure 4: Schematic of ignition quality tester setup [14]

The differential method has been used to determine the start of ignition (SoIgn) in this constant volume combustion chamber. In the conventional method used by the IQT software, the time of start of ignition is defined by the point where the difference in chamber pressure and the initial chamber pressure, defined as P exceeds, a preset value. The default value of this pressure rise used by the IQT system software is 138 kPa. To isolate the effects of the low temperature heat release fuels, the start of ignition as used in this work is defined by the point of intersection of two slopes, the first being the maximum slope during which the chamber pressure increases steeply and the other being the slope of the chamber pressure curve at the pressure recovery point. The pressure recovery point is defined as the point where the chamber pressure regains the initial chamber pressure after drop in pressure due to evaporative cooling as the liquid fuel injected spray breaks down into droplets, evaporates and mixes with the oxidizer in the combustion chamber, detailed information is available in [13] .

The ignition quality of the fuels is determined by analyzing the chamber pressure signal obtained from a piezo-electric pressure transducer. The chamber pressure signal received from the pressure transducer is noisy and requires signal smoothing for accurate data processing and signal was smoothened with local regression using weighted linear least squares and a 2nd degree polynomial model [14].

The Light Naphtha fuel and surrogate fuel, LN_surr, are tested in KR-IQT to investigate their autoignition characteristics in a constant volume chamber. The pressure traces are analyzed to identify the low temperature ignition delay employing procedure explained in the earlier section. Figure 5 represents the summary of comparative study.
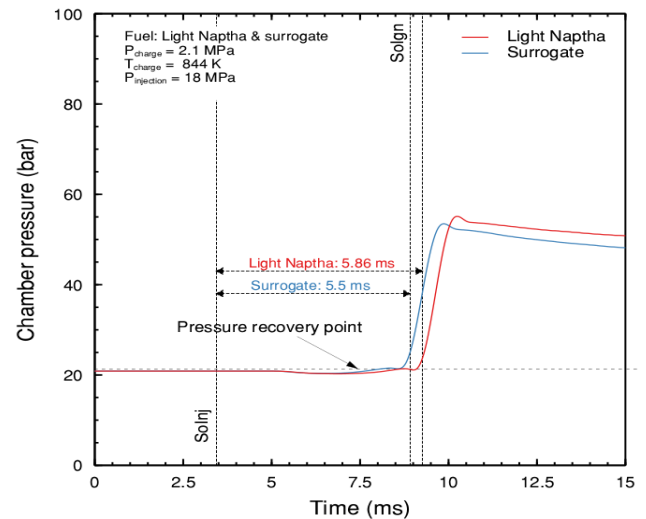

Figure 5: Ignition delay comparison of light naphtha and its surrogate in ignition quality tester

The results of surrogate fuel modeling and KR-IQT data confirm similar physical, chemical and autoignition characteristics of the proposed surrogate fuel developed

in this study. However slightly higher volatility of the surrogate is reflected in the earlier pressure recovery in the IQT experiments, leading to slightly low ignition delay than the light naphtha. This issue could be addressed by having the ADC measured of the light naphtha which will enhance the capability of surrogate to emulate the autoignition.

Conclusions

Overall the proposed surrogate is observed to emulate Light Naphtha fuel closely across various domains.

Acknowledgement

Abbreviations

HCCI: Homogenous compressed charge ignition
PPCI: Partially premixed compression ignition
Vol: volume

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