Fuel 222 (2018) 21–34

Contents lists available at ScienceDirect

Fuel

journal homepage: www.elsevier.com/locate/fuel

Full Length Article

Development of a Diesel Surrogate Fuel Library

Patrick G. Szymkowicz[a,*], Jesús Benajes[b]

[a] Diesel Engine Systems Group, Propulsion Systems Research Lab, GM Global Research & Development, 800 North Glenwood Ave., Pontiac, MI 48340-2925, USA
[b] CMT-Motores Térmicos, Universitat Politècnica de Valencia, Camino de Vera s/n, 46022 Valencia, Spain

ARTICLE INFO

Keywords:
Diesel fuel
Surrogate fuel
Surrogate Fuel Library
Fuel properties
Cetane number
Threshold soot index

ABSTRACT

Diesel fuel is composed of a complex mixture of hundreds of hydrocarbons that vary globally depending on crude oil sources, refining processes, legislative requirements and other factors. In order to simplify the study of this fuel, researchers create surrogate fuels to mimic the physical and chemical properties of Diesel fuels. This work employed the commercial software Reaction Workbench – Surrogate Blend Optimizer (SBO) to develop a Surrogate Fuel Library containing 18 fuels. Within the fuel library, the cetane number ranges from 35 to 60 (in increments of 5) at threshold soot index (TSI) levels representative of low, baseline and high sooting tendency fuels (TSI = 17, 31 and 48, respectively). The Surrogate Fuel Library provides the component blend ratios and predicted properties for cetane number, threshold soot index, lower heating value, density, kinematic viscosity, molar hydrogen-to-carbon ratio and distillation curve temperatures from T_{10} to T_{90}. A market petroleum Diesel fuel with a cetane number of 50 and a threshold soot index of 31 was selected as the Baseline Diesel Fuel. The combustion, physical and chemical properties of the Baseline Diesel Fuel were precisely matched by the Baseline Surrogate Fuel. To validate the SBO predicted fuel properties, a set of five surrogate fuels, deviating in cetane number and threshold soot index, were blended and examined with ASTM tests. Good agreement was obtained between the SBO predicted and ASTM measured fuel properties. To further validate the Surrogate Fuel Library, key properties that were effected by altering the component blend ratios to control cetane number and TSI were compared to a set of five market Diesel fuels with good results. These properties included density, viscosity, energy density and the T_{10} and T_{90} distillation temperatures. The Surrogate Fuel Library provided by this work supplies Diesel engine researchers and designers the ability to analytically and experimentally vary fuel cetane number and threshold soot index with fully-representative surrogate fuels. This new capability to independently vary cetane number and threshold soot index provides a means to further enhance the understanding of Diesel combustion and design future combustion systems that improve efficiency and emissions.

1. Introduction

The internal combustion Diesel engine is a highly-versatile power plant for industrial applications and personal mobility. Diesel engines enjoy advantages in efficiency, specific torque, durability, scalability and fuel adaptability. As a result of its importance to society, researchers continue to gain understanding and explore novel combustion systems while engine development engineers work to introduce new Diesel combustion technologies into production [1–5]. The continuous improvement of Diesel engine performance, fuel economy, and emissions is required to achieve the complex needs of society.

Diesel fuel is composed of hundreds of hydrocarbon species that are not well-characterized. Research has shown that Diesel fuel is primarily composed of four hydrocarbon classes: normal-alkanes, iso-alkanes, cyclo-alkanes and aromatics [6–8]. The aromatic hydrocarbons are classified by the number benzene rings in the molecule. Mono-aromatics have a single benzene ring and polycyclic aromatic hydrocarbons (PAH) contain two or more benzene rings. As a result of this complex and undefined composition, researchers create Diesel surrogate fuels for computational and experimental investigations [9–16]. A surrogate fuel is a simple analog created from a small set of well-defined hydrocarbon species. Often surrogate fuels are designed to mimic a subset of Diesel fuel properties. A fully-representative surrogate fuel is designed to replicate numerous physical, chemical and combustion properties of a full-range petroleum Diesel fuel. Such fuel properties include cetane number, threshold soot index, lower heating value, density, kinematic viscosity, surface tension, distillation temperatures and aromatic content.

Surrogate fuels have many applications including spray characterization, chemical kinetic modeling and combustion simulation [17–20]. The application of single-component surrogate fuels, such as n-heptane for Diesel combustion kinetics [21–23] and n-dodecane for Diesel fuel

* Corresponding author.
E-mail address: patrick.g.szymkowicz@gm.com (P.G. Szymkowicz).

https://doi.org/10.1016/j.fuel.2018.01.112
Received 11 October 2017; Received in revised form 5 January 2018; Accepted 26 January 2018

Nomenclature

°C	degrees celsius
CN	cetane number
CO	carbon monoxide
DIPPR	design institute for physical properties
H/C	hydrogen-to-carbon ratio
HC	hydrocarbons
LHV	lower heating value
molR	mole ratio
NOx	nitrous oxides
NTC	negative temperature coefficient
OH	hydroxyl radical
PAH	polycyclic aromatic hydrocarbons
Φ	equivalence Ratio
SBO	Surrogate Blend Optimizer
TSI	threshold soot index
ZTC	Zero Temperature Coefficient

physical properties [24–26], are well-understood, highly utilized and greatly valued. Through combustion simulation or experimental work, single-component surrogates have played a significant role to expand the fundamental understanding of Diesel combustion. As engineering tools, single-component surrogates have guided the development of conventional and novel Diesel combustion systems. However, single-component surrogates cannot fully represent the physical, chemical and combustion properties of Diesel fuels.

Recent work has increased the number of well-characterized hydrocarbons that are representative of Diesel fuel and potentially useful as surrogate fuel components [8,18,14,27–29]. These efforts have enabled the development of multi-component surrogate fuels that can more closely replicate the properties of Diesel fuel [30,31,15,16,32–36]. However, as researchers strive to match the combustion and physical properties of Diesel fuel, the complexity of multi-component surrogate fuels has greatly increased. Surrogates assembled with numerous components exceedingly raise the expense of analytical and experimental implementation. For successful industrialization, the tradeoffs between surrogate complexities and predictive combustion simulation accuracy must be understood, rationalized and optimized for the intended application.

Additional forces driving researchers include the understanding that fuel supplies and standards vary regionally and that future Diesel fuels may be considerably different from current fuels. Today, Diesel engine manufacturers encounter a broad range of fuel properties that may influence engine design and the introduction of new technologies. For example, in the United States ASTM D975-16a established a minimum cetane number requirement of 40 [37] whereas in Europe EN 590:2009 required a minimum cetane number of 51 [38]. As a result of variations in fuel properties, Diesel combustion researchers and design engineers require surrogate fuels that provide the capability to independently control two key fuel properties: cetane number and threshold soot index [39]. While doing so other essential Diesel fuel properties such as density, viscosity, heating value and distillation curve temperatures must be reasonably controlled within the range of market fuels. It is believed that the systematic application of multi-component surrogate fuels with independent control of fuel cetane number and threshold soot index will enhance the fundamental understanding of combustion, efficiency and emissions. At the same time, improved surrogates may provide a means for future improvements in Diesel spray modeling, combustion simulation, and predictive NOx, CO, HC, soot and exhaust particle emissions.

This investigation creates a library of fully-representative multi-component surrogate Diesel fuels that are appropriate for both exploratory combustion research and direct application to the engine combustion system design process. The effort balanced complexity and accuracy with usefulness and the ability to industrialize the findings.

2. Objective and requirements

The objective of this research was to bring multi-component surrogate fuels closer to routine use by the automotive industry. To this end, the following requirements were placed on the surrogate fuels developed through this investigation:

- The Surrogate Fuel Library must contain a Baseline Surrogate Fuel that closely matches the combustion, physical and chemical properties of a Baseline Petroleum Fuel (market fuel.)
- The Surrogate Fuel Library must contain surrogate fuels with cetane number ranging from 35 to 60 (in increments of 5). In doing so, the library covers potential next-generation fuels which may extend the cetane number range as low as 35 for naphtha-like fuels [40,41] or as high as 60 for synthetic fuels [42,43].
- The library must contain threshold soot index levels representative of low, baseline, and high sooting fuels. Three TSI levels are required to reproduce potential fuel variations and support future investigations that enhance the understanding of soot and particle emissions.
- The combustion and physical properties of the surrogate fuels, namely lower heating value, density, viscosity, surface tension, and distillation curve temperatures, must be representative of market Diesel fuels.
- The number of surrogate fuel components must be kept to a minimum to manage increased complexity, kinetic mechanism size, computational and experimental expenses.
- To support spray and combustion simulation, the combustion, physical, chemical and temperature-dependent properties of the surrogate components must be available along with validated, detailed kinetic mechanisms.
- To support experimental work, the surrogate components must be available with high-purity, in large quantities, and must meet safety guidelines for storage, blending and handling.

3. Methodology

3.1. Master kinetic mechanism

As mentioned above, there has been and continues to be substantial progress in the development of detailed kinetic mechanisms for surrogate fuel components. This work employed the ANSYS 2015 Model Fuel Library and the accompanying Diesel Fuel Master Kinetic Mechanism [44]. The kinetic mechanism consisted of 55 fuel components, 5155 chemical species and 31,084 chemical reactions. The mechanism was accompanied by physical, chemical and thermodynamic properties for the fuel components. The fuel component information was utilized to predict surrogate fuel properties and the kinetic mechanism was used for closed-homogenous gas-phase reactor simulations.

3.2. Surrogate blend modeling and fuel property predictions

A review of the literature revealed several methods to formulate surrogate fuels [9,45–54]. In this work, the Reaction Workbench – Surrogate Blend Optimizer (SBO) was employed to model surrogate fuel properties, understand the impact of various compounds on the surrogate properties, determine the blend mixtures needed to achieve the objectives and predict the surrogate properties [52,55]. The SBO utilized a genetic optimization procedure that minimized the differences between user specified fuel properties and their computed values. Upon iteration and convergence, the SBO delivered the surrogate composition