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# Single-cylinder engine evaluation of a multi-component diesel surrogate fuel at a part-load operating condition with conventional combustion

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ABSTRACT

Simple, yet fully-representative surrogate fuels are needed to model market Diesel fuels. The surrogates must closely mimic market Diesel fuel properties and match the engine combustion and emissions behavior. To this end, the combustion and emissions performance of a market Diesel fuel and a four-component surrogate fuel were investigated using a single-cylinder, light-duty Diesel engine with contemporary combustion and fuel injection technology. The surrogate fuel, which was developed in previous work, was composed of normal-hexadecane/2,2,4,4,6,8,8-heptamethylnonane/decahydronaphthalene/1-methylnaphthalene with a volume fraction formulation of 0.37/0.33/0.18/0.12. Fuel test results showed the physical, chemical and combustion properties of the market Diesel fuel were closely matched by the surrogate. The fuels were evaluated by engine tests conducted at 1500 r/min and 9 bar IMEP. At this operating condition, the Diesel combustion process demonstrated low-temperature heat release, premixed and diffusion combustion regions. Test results from EGR and combustion phasing sweeps showed the engine combustion behavior, exhaust CO, HC, NOx, smoke and particle size distributions from the market Diesel fuel were very closely matched by the surrogate fuel. It can be concluded that under the engine conditions evaluated by this work, the four-component surrogate fuel accurately represents the market Diesel fuel. Thus, for conventional Diesel combustion conditions, the surrogate should prove useful for future applications such as kinetic mechanism development, fuel spray and combustion simulation, and further experimental investigations.

## 1. Introduction

To efficiently develop advanced Diesel combustion systems, practical spray and combustion models are needed that quantitatively predict engine combustion and emissions. Within this framework, accurate chemical kinetic models are needed to predict low temperature reactions, auto ignition, heat release, exhaust emissions, and soot. Given the complexity of market Diesel fuels, simple surrogate fuels are used to model the physical, chemical and combustion properties of Diesel fuel [1–5]. Assuming that detailed kinetic mechanisms are available for each surrogate fuel component, kinetic mechanism can be assembled and validated for the surrogate fuel. The temperature dependent properties of the surrogate are often modeled using correlations developed by the Design Institute for Physical Properties [6]. Applying this procedure, it is possible to formulate fully-representative surrogate fuels that accurately replicate the physical, chemical and combustion properties of the market Diesel fuel. Single-component surrogates have been used sometimes, but in general, multi-component surrogate fuels are required to fully represent the properties of a market Diesel fuel [7–10].

Examples of single-component surrogate fuels include n-heptane to model combustion kinetics [11–13] and n-dodecane to model fuel physical properties [14–16]. Through combustion simulation or experimental research, single-component surrogates have significantly expanded the fundamental understanding of Diesel combustion. However, single component surrogates can only mimic a limited number of fuel properties. Additionally, they cannot be tailored to replicate the differences observed in market fuel properties such as global variations in Diesel fuel cetane number.

To improve the sooting tendency of single-component surrogates, researchers employed binary surrogates that combined a normal-alkane with an aromatic species. For example, a surrogate known as IDEA fuel was developed that contained 70% n-decane and 30% 1-methylnaphthalene (by volume) [17]. Other examples of binary surrogate fuels include n-heptane and toluene (various mixtures) [5] also 77% n-dodecane and 33% m-xylene [18].

Exceptional progress has been made increasing the availability of kinetic mechanisms for numerous hydrocarbon species [7,19,20]. As a

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**Nomenclature**

| | |
|---|---|
| A/F | air-to-fuel ratio |
| ASTM | American Society for Testing and Materials |
| aTDC | after top dead center |
| °C | degrees celsius |
| CA50 | crank-angle of 50% mass burned |
| CMD | count median diameter |
| CN | cetane number |
| CO | carbon monoxide |
| $CO_2$ | carbon dioxide |
| Dp | particle diameter |
| EGR | exhaust gas recirculation |
| EI | emission index |
| FSN | filter smoke number |
| HC | hydrocarbons |
| HTHR | high temperature heat release |
| IMEP | indicated mean effective pressure |
| LTHR | low temperature heat release |
| molR | mole ratio |
| N | number of particles |
| N/cc | particle number concentration |
| NOx | nitrous oxides |
| $O_2$ | oxygen |
| SOE | start of energizing time of fuel injector |
| TSI | Threshold Soot Index |

result, researchers are developing multi-component surrogate fuels that more closely match Diesel and jet fuel properties. For example, Johnson et al., investigated the auto ignition properties of jet fuels and simple surrogate fuels using a Cooperative Fuel Research (CFR) Diesel engine [21]. For the conditions investigated, the results showed that a four-component surrogate closely matched the auto ignition characteristics of a JP-8 jet fuel. Poon et al. developed a four-component Diesel surrogate that consisted of n-hexadecane, heptamethylnonane, cyclohexane and toluene. Detailed and reduced chemical mechanisms were generated and evaluated with zero-dimensional chemical kinetic simulations and then used to study two-dimensional spray combustion [22,23]. To support chemical kinetic modeling Mueller et al., formulated a set of multi-component surrogate fuels ranging from four components up to nine components. The four-component surrogate consisted of n-hexadecane, heptamethylnonane, trans-decalin and 1-methylnaphthalene [8]. Their proposed surrogates were able to mimic the physical properties of the target fuel, but they were not tested in engine combustion conditions.

With the intent to industrialize the use of multi-component surrogate fuels by the automotive industry, the authors of the present study developed a Diesel Surrogate Fuel Library that consisted of 18 surrogate fuels [9,10]. The surrogates were developed adhering to a set of practical requirements to enable the immediate application of the surrogates. The library provided the surrogate formulations 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 $T_{90}$. Within the library, the fuel cetane number ranged 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 predicted physical, chemical and combustion properties of the surrogates were validated and found to be within the range of properties measured from a set of five market fuels. The properties of the baseline market Diesel fuel with a cetane number of 50 and a TSI value of 31 were precisely replicated by the baseline surrogate fuel (labeled as CN50_TSI31).

However, the diesel combustion is a heterogeneous and transient phenomenon, much more complex than the processes used for testing the fuel properties (like the cetane number or the smoke point). Hence, even though the surrogate fuel would exhibit very similar properties as those of the market fuel, the question remains as up to which extent both fuels would produce similar results in a real combustion process.

Consequently, the current work explored the engine combustion and emissions response of the market Diesel and CN50_TSI31 surrogate fuels in a single-cylinder Diesel engine operating in variable in-cylinder conditions. Compared to multi-cylinder engine testing, single-cylinder engine tests provided a means for excellent control and reproducibility of the operating conditions [24]. To thoroughly examine the fuels, a part-load operating condition was selected that demonstrated low-temperature heat release, premixed and diffusion combustion regions. Both fuels were subjected to the complex physical processes that occur within the Diesel spray, atomization, evaporation and fuel-air mixture formation [15,25–27,14,28]. Conventional Diesel combustion is exceedingly complex [29–31] and encounters rich and lean local conditions that promote soot and NOx formation, respectively [32–34]. In-cylinder soot formation and oxidation is also a complicated process [35,36]. Thus, transitioning the engine from low soot to high soot operating conditions would provide an excellent assessment of the surrogate fuel. NOx formation is also dependent on local equivalence ratio and temperature. To reproduce the NOx emissions from the market Diesel fuel, the surrogate must provide equivalent heat release, local temperatures and local equivalence ratios.

In addition to examining the surrogate fuel, this effort was conducted to assess the hypothesis that closely matching the physical, chemical and combustion properties of a market fuel can provide a practical and effective surrogate even though the particular hydrocarbon species that composes the surrogate may be sparsely present, or not present, in the market Diesel fuel.

## 2. Experimental methodology

### 2.1. Fuels

In previous work, the authors of the present study selected a market Diesel fuel with a cetane number of 50 and a TSI value of 31 then developed a four-component surrogate fuel that closely matched the physical, chemical and combustion properties of the Diesel fuel [9,10]. The four components included n-hexadecane to represent the n-alkane class, 2,2,4,4,6,8,8-heptamethylnonane to represent the iso-alkane class, decahydronaphthalene to represent the cyclo-alkane class, and the aromatics were represented by 1-methylnaphthalene. The volume fractions for the surrogate components were: n-hexadecane = 0.37, heptamethylnonane = 0.33, decahydronaphthalene = 0.18 and 1-methylnaphthalene = 0.12. Table 1 presents the ASTM measured properties for both fuels. To ensure safe and proper operation of the fuel injection system, a lubricity improver was added to the surrogate fuel (100 ppm).

### 2.2. Engine

The experiments were carried out using a fully instrumented single-cylinder Diesel engine with contemporary combustion and fuel injection technology. The primary engine characteristics are given in Table 2.

### 2.3. Operating conditions

A moderate engine speed and load was used to evaluate the fuels under conventional Diesel combustion conditions. The engine speed was maintained at 1500 r/min and the engine load was held constant at