



## Full Length Article

# Experimental study of autoignition characteristics of Jet-A surrogates and their validation in a motored engine and a constant-volume combustion chamber



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## HIGHLIGHTS

- A good agreement in combustion kinetics of UM II surrogate and Jet-A was verified in a motored engine.
- UM I surrogate showed an advanced ignition behavior as compared to Jet-A in a motored engine.
- Ignition delay for both surrogates showed a comparable trend with Jet-A in constant volume combustion chamber.
- Decalin is a better cycloalkane to use than MCH in the surrogate fuel mixture, due to closer physical properties to Jet-A.

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## ABSTRACT

The current study presents an experimental validation of jet aviation fuel surrogates formulated using a surrogate model-optimizer. Two surrogate fuel mixtures are used to emulate a practical Jet-A (POSF 4658) considering a series of physical and chemical processes in diesel engines. The surrogate mixtures consist of: *n*-dodecane/isocetane/methylcyclohexane (MCH)/toluene 0.3844/0.1484/0.2336/0.2336 on a molar basis (referred to as UM I), and *n*-dodecane/isocetane/decalin/toluene 0.2897/0.1424/0.3188/0.2491 on a molar basis (referred to as UM II). In the present study, a modified Cooperative Fuels Research (CFR) Octane Rating engine and an optically accessible, constant-volume spray combustion chamber are employed to investigate how the chemical and physical properties of these jet fuel surrogate mixtures affect the fundamental ignition behavior as compared to the targeted full boiling range Jet-A fuel (POSF 4658). The observations of ignition behavior include critical compression ratio and critical equivalence ratio, and % low temperature heat release, which are assessed using the motored engine (CFR), while physical and chemical ignition delays are measured using a modified Cetane Rating (CID 510) instrument under a wide range of air temperatures and oxygen dilution levels.

The measured derived cetane number (DCN) for UM I shows a reasonably good match with the practical Jet-A fuel (POSF 4658), while gas-phase oxidation behavior is less, well-matched in the modified CFR engine. In contrast, although the measured DCN of UM II revealed a lower value than the estimated value using a surrogate optimizer, the ignition behavior is relatively well match with that of the target Jet-A in the modified CFR engine. The similarities in physical and chemical ignition delays as compared with the target Jet-A support the effectiveness of the UM II surrogate, while in contrast, the UM I surrogate only matched the chemical ignition delay. This is attributed to the importance of the surrogate component decalin, which improved the physical properties as compared to MCH, while the other three components were the same for the two surrogates.

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## 1. Introduction

Fuel specification standards dictate requirements on a variety of chemical and physical properties of fuels being produced from

petroleum and derived from alternative resources to ensure that the fuels will serve well in their application, for example aviation turbine engines. For aviation turbine fuels, the fuel specification test method, ASTM D7566-14c, ensures that fuels meeting the specification will function effectively in commercial turbine engines [1]. Other tests may be specified beyond the ASTM or military standards, determining hydrocarbon chemistry, bulk physical and performance properties, electrical properties and ground handling/safety, referred to as ‘fit-for-use’ [2]. Jet fuel specifications are designed to govern their use as fuel for aviation gas turbine engines. However, the U.S. Army’s single battlefield fuel policy also mandates the use of JP-8 in ground vehicles employing compression ignition engines for the simplification of supply chain logistics [3].

The combustion process in diesel engines is different from gas turbine engines, given that the onset of combustion in a diesel (compression ignition) engine is mostly governed by an ignition delay period between the start of injection (SOI) and the start of combustion (SOC), wherein complex fuel dependent physical and chemical phenomena play a crucial role. Cetane number (CN) is related to the ignition delay period in the diesel engine combustion process under the ASTM D613 test method [4]. The CN variations for petroleum and non-petroleum derived jet fuels may fall below the minimum CN specification for compression ignition engines, leading to difficulties in engine starting, and performance [5]. To overcome this critical barrier, the development of diesel engine combustion simulations with computational fluid dynamics (CFD) is needed to support an understanding of how physical and chemical properties of practical jet fuels affect the ignition delay.

Since practical jet fuels may be comprised of hundreds of hydrocarbon molecules, the development of validated, predictive and multi-scale combustion models is a challenge to implement with limited ability to use detailed reaction chemistry in conjunction with detailed engine CFD simulations. Therefore, practical simulation of the diesel engine combustion process requires the use of simplified chemical kinetic models and the consideration of model compounds or mixtures of model compounds, referred to as surrogate fuels [6]. In a diesel engine, liquid fuel is directly injected into the combustion chamber and prepared for ignition by various physical and chemical process. To be useful for capturing combustion behavior within diesel engines, the surrogate fuels for the diesel engine combustion process must successfully emulate the physical properties and gas-phase combustion behavior of the target fuel with a limited number of pure components.

In recent decades, much work has addressed the formulation of aviation fuel surrogates and their chemical mechanisms have been reported with experimental validation in simplified combustion chambers such as shock tubes [7–12], rapid compression machines (RCM) [9,10,12], pressurized flow reactors (PFR) [9–12], jet-stirred reactors (JSR) [12,13] and co- and counter flow burners [9,10,12,14,15]. Furthermore, recent kinetic modeling studies validated ignition characteristics of jet fuel surrogates in a wide range of conditions by using compact multi-component chemical reaction mechanisms [16,17]. The resultant surrogate developments are important from a point of view of accurate chemical kinetic predictions, as compared to real jet fuels. However, these studies mainly deal with emulating combustion kinetics of gas-phase fuel/oxidizer mixtures, generally matching chemical properties such as derived cetane number (DCN), hydrogen to carbon ratio (H/C), molecular weight (MW), and threshold sooting index (TSI) but no effort is made to match the temperature-dependent physical properties of a real jet fuel. Meanwhile, Edwards and Maurice stressed the importance of considering the physical properties (e.g., distillation curve, viscosity, density, surface tension, etc.) of surrogates over a wide range of pressures and temperatures [18]. Bruno et al. also investigated thermal physical properties of Jet-A

and S8, with matching surrogate models [19,20]. However, replicating the detailed physical properties of a real jet fuel generally requires larger numbers of components of varying molecular weights. For instance, a few previous studies have adopted 7–14 pure components to match the aforementioned physical properties of a practical jet fuel [18,21]. However, the use of a larger number of surrogate components creates challenges to develop tractable gas-phase combustion kinetics. For this reason, most recent work has favored emulating the fully gas-phase global combustion behavior with fewer (from 1 to 4) surrogate components. It is important to consider both, physical and chemical properties of real fuels, as pointed out by other studies [10,11]. Combined emulation of physical and chemical properties becomes more crucial in development of comprehensive models for the diesel combustion process, where the ignition delay period, the premixed combustion phase, mixing controlled combustion or the diffusion burn phase, and the late combustion phase occur consecutively [22].

Heywood reviewed the significant impacts of surface tension and liquid density on physical processes that affect a diesel spray, while volatility and viscosity play minor roles in ignition delay in a warmed up engine [22]. Caton et al. suggested several ignition delay correlations with respect to physical properties by using various pure component fuels in a single cylinder diesel engine [23]. Fig. 1 shows a diagram of ignition delay periods, presenting the impacts of physical properties such as liquid density, liquid viscosity, surface tension, and vapor pressure on preparation of liquid fuel after the liquid fuel jet is injected in the combustion chamber. Once the fuel and air are premixed with a given mixture ratio at suitable temperatures and pressures, there is a chemical delay period where chemical reaction rates promote and ultimately lead to significant chain branching. The rates of fuel decomposition mainly rely on the molecular structure such as chain length, presence of double- or triple-bonds, degree of branching, cyclic or aromatic structure and substitution of oxygen or other species, as shown in Fig. 1. During fuel decomposition, an alkyl peroxide isomerization step is considered as the key reaction step for predicting the onset of ignition under low and intermediate temperature regimes usually observed in advanced diesel combustion systems [24]. Furthermore, the molecular weight (MW) affects the liquid/vapor phase diffusive transport of fuel species and the lower heating value (LHV) determines the energy that can be released through the oxidation of the fuel. Finally, the local air/fuel ratio and adiabatic flame temperature are influenced by the H/C ratio during the premixed combustion phase.

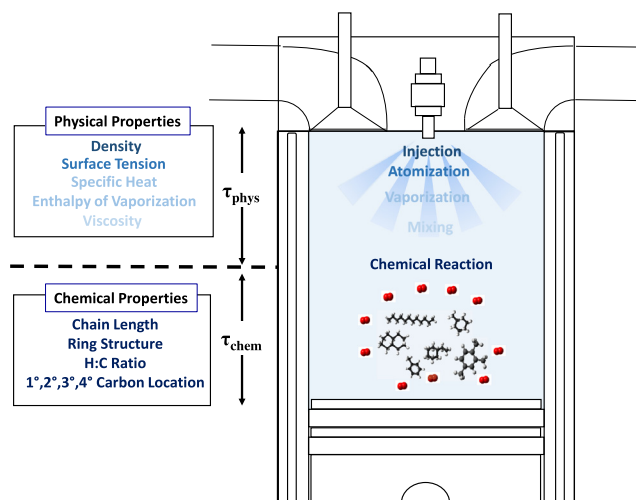


Fig. 1. Physical and chemical properties affecting diesel engine combustion processes, inspired by [23].

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