# A surrogate for emulating the physical and chemical properties of conventional jet fuel

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## ARTICLE INFO

## ABSTRACT

Two surrogates are developed using a model-based optimizer to emulate the fuel properties affecting the spray development and gas phase ignition of a conventional jet fuel. The first surrogate, UM1, is a mixture of n-dodecane/iso-cetane/methylcyclohexane/toluene (0.3844/0.1484/0.2336/0.2336 mol fraction), while the second, UM2, is a mixture of n-dodecane/iso-cetane/decalin/toluene (0.2897/0.1424/0.3188/0.2491 mol fraction). The developed surrogates contain hydrocarbon species that are available in existing chemical mechanisms, and emulate both the physical and chemical properties of a representative real jet fuel, Jet-A POSF-4658. POSF-4658 is suitable as a surrogate target fuel since the properties of POSF-4658 are representatives of a nominal Jet-A, and a wide range of experimental POSF-4658 data is readily available, including multiple ignition delay measurements. While the UM1 surrogate gives a much tighter match for temperature-independent properties, UM2 is shown to better emulate liquid density and volatility, properties which are known to be important to spray predictions under engine relevant conditions. The new UM surrogates improve upon emulation of the chemical and physical properties of POSF-4658 compared with surrogates that currently exist in the literature. Ignition delay times predicted with a detailed chemical mechanism and the newly developed surrogate compositions under diesel relevant conditions show reasonable agreement with shock tube and rapid compression machine experiments.

## 1. Introduction

The U.S. Army's single fuel forward policy mandates the use of JP-8 in deployed aircraft, ground vehicles and equipment for the simplification of supply chain logistics [1]. As a result, the Army's diesel engines must be capable of operating with JP-8, which is quite similar to commercial aviation kerosene Jet-A-1. Gas turbines and jet engines are the main consumers of JP-8, and combustion within these devices is only marginally affected by the auto-ignition characteristics of fuel, which is measured by the cetane number (CN). The resulting lack of CN specification for petroleum derived JP-8 can result in CN ranging from 36 to 50 [2]. The mean CN variation becomes even more drastic with non-petroleum derived jet fuels, where with coal-derived jet fuel (SASOL IPK) CN can be on the order of ∼31 [3], while the CN of a natural-gas-derived jet fuel (S8) is ∼60 [4].

Typically, the onset of combustion in diesel engines is controlled through the injection timing, where the period between the start of injection (SOI) and the start of combustion (SOC) is

known as the ignition delay. It is well known that the ignition delay period is governed by complex fuel dependent physical and chemical phenomena, which prepare the stratified fuel–air charge for combustion [5]. Considering that the CN of the fuel can influence the length of the ignition delay, the use of JP-8 in diesel engines calibrated for diesel fuel can be challenging [6], as ignition can range from instantaneous ignition to no ignition at all. While engine experiments enable some global understanding of this behavior through heat release analysis, an understanding of how these physical and chemical phenomena affect the ignition delay is quite limited. Diesel engine combustion simulations with Computational Fluid Dynamics (CFD) are therefore able to complement metal engine experiments with insight into spray and gas phase combustion behavior.

Real fuels are often composed of hundreds to thousands of molecules, and the use of such a large number of species is beyond the current reach of engine level CFD applications. Therefore, surrogate fuels and their associated chemical mechanisms have been developed and utilized to model the oxidation process of a real fuel within CFD simulations. To be useful for combustion within practical devices, the surrogates must successfully emulate the targeted properties and combustion behavior of the real fuel with a handful of well-characterized pure components. Targets for the

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surrogate formulation differ depending on the intended application of the surrogate.

Previous efforts, including surrogate formulation, chemical mechanism development and experimental data for validation prior to 2007 are extensively reviewed in [7] for gasoline, [8] for diesel, and [9,10] for jet fuel. Vasu et al. [11] evaluated a number of surrogates and mated mechanisms by comparing calculated ignition delays against real jet fuel shock tube data. The results showed that the Violi surrogates [12] coupled with the Ranzi mechanism [13] gave the closest ignition delay predictions among the tested surrogates/mechanisms at temperatures above 1000 K; low temperature ignition delays were not well-predicted. More recently, the critical conditions for the auto-ignition and extinction of several jet fuel surrogate mixtures were experimentally evaluated in [14]. Among the tested mixtures, the UCSD surrogate (n-dodecane/methylcyclohexane/o-xylene) and the Aachen surrogate (n-decane/1,2,4-trimethylbenzene) best reproduced the experimental data of real JP-8. The critical conditions of auto-ignition for the UCSD surrogate [15] and for the Aachen surrogate [16] were calculated using chemical mechanisms and agreed well with experimental measurements. Dooley et al. [17] formulated a jet fuel surrogate composed of n-decane/iso-octane/toluene which reproduced the CN and Hydrogen–Carbon ratio (H/C) of a representative Jet-A, POSF-4658. The gas phase combustion characteristics of the surrogate were experimentally validated in various devices as well as with simulations. More recently, their 2nd generation surrogate [18], which is a mixture of n-dodecane/iso-octane/1,3,5-trimethylbenzene/n-propylbenzene, was capable of reproducing the CN, H/C, Molecular Weight (MW) and Threshold Sooting Index (TSI) of the same target fuel, while ignition modeling studies with the surrogate were conducted in [19]. Naik et al. [20] formulated surrogates (n-decane/n-dodecane/iso-octane) for Fischer–Tropsch (F–T) jet fuels derived from natural gas and developed a chemical mechanism for their surrogates. When compared to previous surrogates that were designed to mimic conventional jet fuels, the Naik et al. surrogates do not include any cycloalkane or aromatic components since F–T jet fuels are composed mostly of lightly branched iso-alkanes and straight n-alkanes. While all the surrogates mentioned above were targeted to mimic gas phase combustion characteristics and agreed reasonably well with experimental data, little or no consideration were given to temperature dependent physical properties in the liquid phase, which are known to affect spray breakup, evaporation, and molecular diffusion [18,21,22]. While surrogates from NIST emulated the various temperature dependent physical properties and CN of conventional jet fuels [23] and the F–T jet fuel S-8 [24], the molecules of the NIST surrogates lack chemical mechanisms, making their use in CFD problematic.

In order to address the need for a jet fuel surrogate for CFD application that is capable of capturing both physical and chemical processes during the diesel ignition delay period, the current work reports the development of surrogate mixtures that emulate the physical and chemical properties of conventional jet fuel. Starting with the properties known to affect mixture preparation and gas phase ignition within diesel engines, eight target properties were chosen for the formulation of new jet fuel surrogates, which were CN, MW, lower heating value (LHV), H/C ratio, density, viscosity, surface tension, and distillation characteristics. The surrogates were developed with only those species readily available in existing kinetic mechanisms. The resulting properties of the newly developed jet fuel surrogates were compared to the properties of real jet fuel and existing surrogates. Additionally, surrogate performance assessment was performed by comparing the calculated gas phase ignition delay to the measured ignition delay times of the conventional jet fuel in shock tubes and rapid compression machines (RCM).

## 2. Surrogate formulation methodology

### 2.1. Selection of surrogate target properties

The diesel combustion process is composed of several phases, including the ignition delay period, the premixed combustion phase, the mixing-controlled combustion or diffusion burn phase, and the late combustion phase [5]. The liquid fuel jet injected into the combustion chamber is prepared for ignition by a series of physical and chemical processes during the ignition delay period [25]. Initially, the liquid phase of the fuel jet breaks down, generating small liquid droplets. This process is affected by the charge density, fuel jet momentum, and the liquid fuel physical properties. Next follows the evaporation of the fuel droplets, which is a strong function of the charge temperature and the liquid fuel volatility as measured by the vapor pressure. Finally, the vaporized fuel is mixed with air to help create the combustible fuel/air mixture. This fuel/air mixing process depends on physical factors such as turbulent mixing, thermal and compositional gradients as well as species diffusivities. Within IC engines, geometric factors, such as combustion chamber/piston bowl design and injector design can also affect the combustion process. In order to model these complex physical processes, a series of phenomenological/physical models have been developed and used within a variety of computational studies [25]. These spray sub-models include physical properties of the liquid phase fuels as model parameters such as density, viscosity, surface tension, and vapor pressure [25,26]. Thus, the characteristics predicted by the spray model are expected to be a function of the physical properties of the surrogate fuel, in addition to the assumptions for the droplet distribution.

At the same time, the chemical processes which prepare the fuel–air charge for ignition are enhanced by the high temperatures and pressures within the combustion chamber. Decomposition of the fuel molecules into smaller hydrocarbons and active radicals initiates the spontaneous ignition of the fuel–air charge which is properly mixed, leading to the premixed combustion phase. This process is affected by fuel properties, including the ignitability of the fuel, often represented by CN for diesel applications. The MW affects the liquid/vapor phase diffusive transport of fuel species, while the 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.

In order to properly address the dependency of the diesel ignition processes on various liquid fuel properties, eight properties were chosen as target properties for the surrogate as shown in Table 1. Three of the property targets are chemical in nature, including CN, LHV and H/C. MW is a temperature independent physical property. Also, three temperature dependent physical

**Table 1**
Eight surrogate target properties for the target fuel POSF-4658 and weights assigned to each target properties for the optimization process (Eq. (1)).

| Target properties | Measured values | Weight ($w_i$) | |
|---|---|---|---|
| | | UM1 | UM2 |
| CN | 47.1 (DCN[a]) [17] | 10 | 10 |
| LHV | 43.23 MJ/kg [33][b] | 10 | 2 |
| H/C | 1.957 [17] | 10 | 10 |
| MW | 142 kg/kmol [17] | 10 | 20 |
| Density | Temperature-dependent [32] | 0.5 | 2 |
| Viscosity | Temperature-dependent [32] | 0.5 | 10 |
| Surface tension | Temperature-dependent [34][c] | 0.5 | 0.6 |
| Distillation curve | [31] | 0.5 | 2 |

[a] Derived cetane number.
[b] The mean of JP-8 samples in 2009.
[c] The surface tension for Jet-A, Jet-A-1, and JP-8.