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Development of a new jet fuel surrogate and its associated reaction mechanism coupled with a multistep soot model for diesel engine combustion

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HIGHLIGHTS

- A new jet fuel surrogate was developed by emulating real jet fuel properties.
- A jet fuel skeletal reaction mechanism coupled with a multistep soot model was developed.
- Mechanism validations of ignition delay times, species concentrations and laminar flame speed were done.
- Validations in a constant volume chamber and an engine showed the reasonableness of this mechanism for application.

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ABSTRACT

A new jet fuel surrogate was developed in this work by emulating real jet fuel properties including physical, gas phase chemical properties and threshold sooting index (TSI). An intelligent optimization methodology was proposed to calculate the species composition that inherently satisfies both the physical and chemical characteristics as well as sooting tendency. Eight properties were selected as the target properties for the jet fuel surrogate development, including liquid density, viscosity, surface tension, cetane number (CN), hydrogen carbon (H/C) ratio, molecular weight (MW), lower heating value (LHV) and TSI. As a result, the CN, H/C ratio, LHV, TSI and density of the new jet fuel surrogate are reproduced excellently with very little deviations within 3%. The averaged deviation of viscosity is −6.318% and the deviations of MW is 9.776%. As the highest deviation among all properties, the averaged deviation of surface tension is 11.76%. Based on the newly developed jet fuel surrogate, a skeletal jet fuel surrogate mechanism with 5 components including decalin, *n*-dodecane, *iso*-cetane, *iso*-octane and toluene was developed. The skeletal jet fuel surrogate mechanism was significantly compacted into 74 species and 189 reactions by describing the chemistries for the oxidation of large molecules C_4–C_n and small H_2/CO/C_1 molecules respectively, which makes it practical to be used for 3-D engine combustion simulations. The validations of ignition delay times present reasonable agreement between experiment and predictions over a wide range of equivalence ratios (0.5–2.0) and pressures (8–30 atm), except for a shift of negative temperature coefficient (NTC) region towards higher temperatures at $\Phi = 1.5$, 20 atm: in the simulation the NTC region is from 830 K to 950 K while in the experiment the NTC region is from 740 K to 890 K. The predicted species concentrations can reproduce the trend of the experimental data, especially for O_2, CO and CO_2. The simulated laminar flame speed at 400 K and 470 K are with absolute averaged deviations of 3.5% and 4.06% respectively. The constant volume spray and combustion validations are reasonably good. In the engine combustion validations, a multistep soot model was embedded into the new jet fuel surrogate mechanism. The predicted in-cylinder pressure can reproduce the experimental data, expect for small deviations after the peak pressure (the averaged deviation is around 6.2% after the peak pressure). The embedded soot model can well reproduce the trend of the experimental data. It can be concluded that this new jet fuel surrogate mechanism is compact and robust for the utilization in diesel engine combustion simulation.

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Nomenclature

V_i	volume fraction of component i
X_i	mole fraction of component i
H_i	the number of hydrogen atoms of component i
C_i	the number of carbon atoms of component i
Y_i	the mass fraction of component i
T	liquid temperature

1. Introduction

Jet fuel is one of the most important class of fuel for transportation which is widely used in industry. Jet fuels such as Jet-A and Jet-A-1 were used for civil aviation, while the military aircraft was fueled with JP-8 which is rather similar to Jet-A [1]. Also, jet fuel was becoming more and more popular for utilization in diesel engines of generators and ground vehicles [2]. One of the most significant driving forces is the army's single fuel forward policy for the simplification of supply chain logistics [3]. In addition, the fact that the adulteration of diesel with jet fuel is very common in some regions of the world is another reason which cannot be neglected [4]. Lee et al. [2] also showed the potential of NOx and PM reduction by the optimized JP-8 combustion comparing to that of conventional diesel, as shown in Fig. 1. As such, the investigations on the utilization of jet fuel in diesel engines are becoming necessary.

The real jet fuel is actually composed of thousands of species. With such a large amount of species, it is not practical to carry out the engine level computational fluid dynamics (CFD) applications. As such, the surrogates of real jet fuel and its associated chemical reaction mechanisms have been studied and used to reproduce the combustion process of the real jet fuel by CFD simulations. In order to perform the combustion simulations accurately, the jet fuel surrogate must be capable of emulating the target properties and the combustion characteristics of the real fuel.

Many researchers have been making great efforts to formulate jet fuel surrogates, to develop chemical mechanisms and to carry out experiments on jet fuel. In 2002, Violi et al. proposed a jet fuel surrogate mixed with six pure hydrocarbons [5] coupled with a mechanism form Ranzi [6] (*m*-xylene, *iso*-octane, MCH, *n*-dodecane, *n*-tetradecane, tetralin) and (*n*-octane, *n*-dodecane, *n*-hexadecane, xylenes, decalin/tetralin). The validation of jet fuel shock tube experiment done by Vasu et al. [7] showed that this six components mixed mechanism can capture the ignition delay times at temperatures above 1000 K, however showed large errors at low temperatures. In 2005, Daguat and Cathonnet [1] reported that many jet fuel surrogate mechanisms were only validated for species concentrations at low pressure conditions which are not engine relevant conditions. In 2006, Dagaut et al. [8] reported four different jet fuel surrogate mechanisms for combustion simulation, wherein a surrogate with three components (*n*-decane, *n*-propylbenzene and *n*-propylcyclohexane) performed the best under the conditions of jet stirred reactors. In 2007, Gokulakrishnan et al. [9] proposed a detailed mechanism with four components (*n*-decane, *n*-decene, *n*-propylcyclohexane and npropylbenzene) for gas turbine combustion simulation. With this mechanism, the species concentrations were well captured in a jet stirred reactor, while ignition delay times were not validated extensively. In 2009, Honnet et al. [10] proposed a so-called Aachen surrogate mechanism containing two major components (*n*-decane and 1,2,4 trimethylbenzene), which can well reproduce the critical conditions of auto-ignition of jet fuel. In 2010, Dooley et al. [11] developed a jet fuel surrogate (1st generation MURI) composed of three components (*n*-decane, *iso*-octane and toluene), which captured CN and H/C of jet fuel. Both experiment and simulations were performed for validating the combustion characteristics of this jet fuel surrogate. In 2012, Dooley et al. [12] proposed an improved jet fuel surrogate (2nd generation MURI) containing four components (*n*-dodecane, *iso*-octane, *n*-propylbenzen and 1,3,5-trimethylbenzene), which can capture the jet fuel target properties of CN, H/C, MW and TSI. The simulation studies for ignition characteristics with this surrogate were carried out by Malewicki et al. [13] in 2013, which indicated that the 2nd generation MURI model was able to predict the mole fractions of the fuel components, O_2, CO, CO_2 and the C1–C3 hydrocarbons in good agreement with the experimental data. In 2014, Kim et al. [14] developed two model-based surrogates UM1 (*n*-dodecane, *iso*-cetane, methylcyclohexane and toluene) and UM2 (*n*-dodecane, *iso*-cetane, decalin and toluene), which reproduced both physical and chemical jet fuel target properties to some extent. In the same year of 2014, Kavuri et al. [15] proposed a jet fuel surrogate with two components (*n*-heptane and *iso*-octane). This jet fuel surrogate has the same cetane number with the real jet fuel, but the ignition delay times were not successfully validated with the experiments in a shock tube.

Based on the comprehensive review above, although so many jet fuel surrogates were developed to mimic the combustion characteristics, but some flaws do still exist: Firstly, few jet fuel surrogates can well reproduce the physical properties, chemical properties and TSI value of the target jet fuel simultaneously. Secondly, only quite a few jet fuel surrogate mechanisms have performed comprehensive validations against both ignition characteristics and species concentration profiles. Thirdly, most of jet fuel surrogate mechanisms were detailed mechanisms, which were very large and not practical to be used in the 3-D engine combustion simulations. Finally, hardly any researchers embedded a detailed soot model into jet fuel mechanism for engine combustion investigation.

In order to deal with the mentioned problems above and to address the demand for a jet fuel surrogate for engine level CFD applications, the new jet fuel surrogate was proposed and its associated mechanism embedded with a multistep soot model was developed along with systematic validations: (1) accurate and comprehensive emulations for physical properties, chemical properties and TSI value of the target jet fuel, (2) 0-D validations against the experimental data of ignition delay

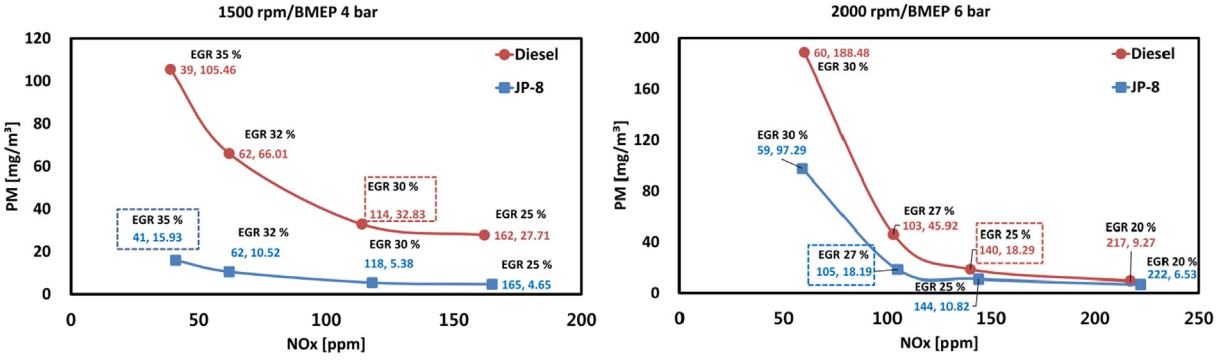

Fig. 1. Potential of NOx and PM reduction by the optimized JP-8 combustion comparing to that of conventional diesel [2].