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Development of an optimization methodology for formulating both jet fuel and diesel fuel surrogates and their associated skeletal oxidation mechanisms

Wenbin Yu, Feiyang Zhao*, Wenming Yang*, Kunlin Tay, Hongpeng Xu

Department of Mechanical Engineering, National University of Singapore, 9 Engineering Drive 1, Singapore 117575, Singapore

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ABSTRACT

In this study, an optimization methodology was developed for formulating both jet fuel and diesel fuel surrogates along with their associated skeletal oxidation mechanisms. Based on this methodology, new jet fuel surrogate (JFS) and diesel fuel surrogate (DFS) are formulated with same five components (n-dodecane/*iso*-octane/*iso*-cetane/decalin/toluene) by emulating practical fuel properties including liquid density, viscosity, surface tension, cetane number (CN), hydrogen-carbon (H/C) ratio, molecular weight (MW), lower heating value (LHV) and threshold sooting index (TSI). Based on the newly developed JFS and DFS, their associated chemical skeletal mechanisms were developed, which are described with same chemical reaction structure: five skeletal sub-mechanisms are employed into the skeletal fuel mechanisms, including decalin ($C_{10}H_{18}$), n-dodecane ($C_{12}H_{26}$), *iso*-cetane ($C_{16}H_{34}$), *iso*-octane (C_8H_{18}) and toluene (C_7H_8) sub-mechanisms. By describing the chemistries for the oxidation of large molecules C4-Cn and small H2/CO/C1 molecules respectively, the skeletal mechanisms are significantly compacted into 74 species and 189 reactions, which makes them practical to be used in 3-D engine combustion simulations. In addition to sufficient 0-D validations of ignition delay times, species concentrations and laminar flame speed in various environments, 3-D validations of constant volume spray and engine combustion were also performed for the new JFS and DFS skeletal mechanisms. It can be observed that the agreements between the computational results predicted by the present mechanisms and all the experimental data are reasonably good, which proves that the newly proposed JFS and DFS skeletal mechanisms are robust and accurate to be used in engine combustion computational fluid dynamics (CFD) studies.

1. Introduction

As the core part for the modern transportation, jet fuel and diesel fuel are the most commonly used class of fuel in the world. As the main fuel for diesel engines, diesel fuel has always played an important role in the world transportation industry. Jet fuel such as Jet-A and Jet-A-1 are mainly used for civil aviation, while the military aircraft is fueled with JP-8 which is rather similar to Jet-A [1]. It also should be noted that jet fuel is becoming more and more popular for utilization in diesel engines of generators and ground vehicles caused by the driving forces of the army's single fuel forward policy [2].

Both jet fuel and diesel fuel consist of thousands of components and the major components of the two fuels are similar hydrocarbons, such as linear paraffins including n-alkanes and *iso*-alkanes, aromatics and cyclo paraffins including mono cycloalkanes and multi cycloalkanes [3,4]. With such a large amount of components, it is not practical to carry out the engine level CFD studies with practical jet fuel and diesel fuel. Therefore, the jet fuel and diesel fuel surrogates and their associated skeletal chemical reaction mechanisms were used in the engine combustion CFD studies. In order to perform the engine combustion numerical study as accurately as possible, the fuels surrogates and their associated mechanisms must be capable of emulating the target properties and the combustion characteristics of the practical fuels.

Great efforts have been made by many researchers to formulate both jet fuel and diesel fuel surrogates, to develop chemical mechanisms and to do the experiments on the oxidation of jet fuel and diesel fuel. Since 2002, many jet fuel surrogates and mechanisms have been proposed. Violi et al. proposed a jet fuel surrogate and its associated mechanism mixed with six pure hydrocarbons [5] which can well predict the ignition delay times at temperatures above 1000 K [6]. Dagaut et al. [7] reported four different jet fuel surrogate mechanisms for combustion simulation, wherein the one with three components (n-decane, n-propylbenzene and n-propylcyclohexane) performed the best by the experiment in a jet stirred reactor. Gokulakrishnan et al. [8] proposed a

* Corresponding author.
E-mail addresses: mpezf@nus.edu.sg (F. Zhao), mpeywm@nus.edu.sg (W. Yang).

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detailed mechanism with four components (n-decane, n-decane, n-propylcyclohexane and npropylbenzene) which can well reproduce the intermediate species concentrations in a jet stirred reactor. Honnet et al. [9] proposed a so-called Aachen surrogate and mechanism containing two components (n-decane and 1,2,4 trimethylbenzene), which can well reproduce the auto-ignition characteristics of jet fuel under critical conditions. Dooley et al. have proposed jet fuel surrogates MURI1 [10] (n-decane, *iso*-octane and toluene) and MURI2 [11] (n-dodecane, *iso*-octane, n-propylbenzen and 1,3,5-trimethylbenzene) since 2010, wherein MURI2 can successfully capture the practical jet fuel properties of CN, H/C, MW and TSI. Kim et al. [12] developed two model-based jet fuel surrogates UM1 (n-dodecane, *iso*-cetane, methylcyclohexane and toluene) and UM2 (n-dodecane, *iso*-cetane, decalin and toluene), which can well reproduce some of the practical jet fuel properties. As for diesel fuel, some single pure hydrocarbons have been used as the diesel fuel surrogate. N-heptane [13] is one of the most common used diesel fuel surrogate because of its comparable CN with practical diesel fuel and the kinetic model is well validated. N-hexadecane [14] is the another common used diesel fuel surrogate since its molecular weight is quite close to the average value of practical diesel fuel. However, only using one single hydrocarbon cannot fully reproduce the properties of practical diesel fuel. A binary mixture surrogate of diesel fuel containing 64% n-heptane and 36% toluene by weight was proposed with a reduced chemical kinetic mechanism which can reproduce the behaviour of the diesel oxidation under engine low temperature combustion conditions [15]. Chang et al. [16] have proposed a four components (n-decane/*iso*-octane/methylcyclohexane/toluene) diesel fuel surrogate along with skeletal mechanism, which can well reproduce the chemical characteristics of practical diesel fuel oxidation but failed in reproduction of physical properties.

Based on the review above, although many jet fuel and diesel fuel surrogates were developed to reproduce the combustion characteristics of practical fuels, some improvements are still needed: Firstly, few jet fuel and diesel fuel surrogates can well reproduce all the physical properties, chemical properties and TSI value of the practical fuels simultaneously. Besides, only a few jet fuel and diesel fuel surrogate mechanisms have performed comprehensive validations against ignition characteristics, species concentrations and laminar flame speed. Finally, most of jet fuel and diesel fuel surrogate mechanisms are detailed mechanisms, which have very large size and not practical to be used in the 3-D engine combustion simulations. In addition to these, since jet fuel and diesel fuel are similar in composition, it is possible to develop an optimization methodology for formulating both jet fuel and diesel fuel surrogates and their associated skeletal oxidation mechanisms, which will be meaningful and time-saving for numerical study of blend fuel with jet fuel and diesel fuel.

In order to deal with the problems mentioned above, an optimization methodology was developed for formulating both jet fuel and diesel fuel surrogates and their associated skeletal oxidation mechanisms. Systematic validations were conducted for the newly developed JFS and DFS along with their mechanisms: (1) comprehensive emulations for physical properties, chemical properties and TSI value of practical fuels; (2) 0-D validations against the experimental data of ignition delay times, species concentrations and laminar flame speed in a wide range of conditions; (3) 3-D validations of constant volume spray and engine combustion.

2. Development of fuel surrogates

2.1. Target properties of fuel surrogates

The combustion process in compression ignition (CI) engines is complicated and is strongly affected by physical and chemical properties of fuels [17]. The fuel spray, as a crucial physical process which significantly affects the ignition characteristics, is dominated by fuel physical properties including liquid fuel density, viscosity and surface tension. The ignition and combustion are also strongly affected by the fuel chemical properties. The CN of fuel is associated with ignitability and the H/C ratio plays significant role in the local equivalence ratio of fuel/air mixture and temperature of adiabatic flame. The MW is usually considered to be the key factor to the fuel liquid/vapor phase diffusive transport and the LHV dominates the energy released from fuel oxidation. As reported in [18], sooting tendency is one of the important fuel properties and it is need to be considered in the new fuel surrogates development. Therefore, in order to comprehensively take into account the effects of various properties of both jet fuel and diesel fuel on ignition and combustion characteristics, eight properties such as CN, H/C ratio, MW, LHV, TSI, density, viscosity and surface tension are considered for formulating JFS and DFS, as shown in Table 1. In this study, POSF-4658, as a representative of practical jet fuel, is selected as the target jet fuel, for which a wide range of experimental data are available including ignition delay times in shock tubes [6,19] and rapid compression machines [11,20], as well as the report of its chemical composition [21] along with chemical and physical properties [3,10,22]. Similar to the previous study [12], because the measurements of LHV and surface tension of POSF-4658 cannot be found, the LHV of JP-8 [23] is regarded as the target LHV and the surface tension of Jet-A, Jet-A-1 and JP-8 is used as the target surface tension [24]. Besides, US #2, specified by diesel automakers for normal driving conditions, is chosen as the target diesel fuel, while all the target properties can be found in Refs. [25–29].

Table 1
Target properties of practical fuels.

Target properties	Jet fuel (POSF-4658)	Diesel fuel (US #2)
CN*	47.1 [10]	46 [26]
H/C	1.957 [10]	1.84 [26]
MW	142 kg/kmol [10]	194 kg/kmol [27]
LHV	43.23 MJ/kg [30]	42.975 MJ/kg [26]
TSI	21.4 [10]	28 [25]
Density	Temperature dependent [22]	Temperature dependent [28]
Viscosity	Temperature dependent [22]	Temperature dependent [29]
Surface tension	Temperature dependent [24]	Temperature dependent [28]

* The derived cetane number (DCN) of jet fuel measured by ignition quality tester (IQT) is used as CN of jet fuel in this study.

2.2. Candidate components selection for fuel surrogates

Although the petroleum-derived jet fuel and diesel fuel consist of thousands of constituents, they have similar majority of components, including n-alkane, *iso*-alkane, cycloalkane and aromatics. Reported in [3], the jet fuel is mainly composed of linear paraffins including n-alkanes and *iso*-alkanes, whose proportion is around 60%. Aromatics and cyclo paraffins including mono cycloalkanes and multi cycloalkanes comprise the rest components of jet fuel with almost the same proportions of around 20%. Moreover, as stated by Pitz and Mueller [31] and Farrell et al. [32], a diesel fuel surrogate which is comprised of a limited number of representative chemical components can well reproduce the properties of the practical diesel fuel. In this study, the selection of candidate components for formulating jet fuel and diesel fuel surrogates is based upon four considerations:

(1) We considered the correlation between candidate components and real fuels in terms of molecular size and H/C ratio.
(2) We also took into consideration the existence of available (skeletal) chemical mechanism(s) that are capable of predicting the oxidation of pure candidate fuel component(s) or whether it is possible to develop the (skeletal) chemical mechanism(s) for the needed fuel candidate components by ourselves.
(3) We also looked at selecting the components which have been extensively used in other jet fuel and diesel fuel surrogate studies.