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An optimization method for formulating model-based jet fuel surrogate by emulating physical, gas phase chemical properties and threshold sooting index (TSI) of real jet fuel under engine relevant conditions

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ABSTRACT

Two jet fuel surrogates (S1 and S2) were proposed in this work, aimed at improving the quantitative accuracy of fuel properties that affect both premixed and spray-guided combustion modes under engine relevant conditions by emulating real jet fuel properties including physical, gas phase chemical properties and threshold sooting index (TSI). An intelligent optimization approach was employed to calculate the composition that inherently satisfies both the physical and gas phase chemical characteristics as well as sooting tendency. The jet fuel surrogate S1 was composed of five components including decalin, n-dodecane, iso-cetane, iso-octane and toluene (0.005/0.4011/0.1249/0.098/0.371 by mole fraction), while surrogate S2 is a mixture of the same components but different in proportions (0.1449/0.3706/0.2059/0.0195/0.2591 by mole fraction). Based on the newly proposed surrogates, a skeletal jet fuel surrogate chemical reaction mechanism was developed by describing the chemistries for the oxidation of large molecules C_4–C_n and smaller H_2/CO/C_1 molecules respectively. The skeletal jet fuel surrogate mechanism was significantly compacted into 74 species and 189 reactions, making it practical to be used in 3-dimensional (3-D) engine combustion simulations. This newly developed mechanism was verified against the experimental results of ignition delay times, species concentrations and laminar flame speed under a wide range of conditions, while 3-D validations were conducted for spray liquid and vapor penetrations in a constant volume chamber. As a result, the proposed fuel surrogate is capable of predicting the spray and combustion characteristics and main species profiles under engine relevant circumstance. Due to the stringent target properties used in this work, the surrogate S1 performed best in assessing ignition characteristics attributed to its elaborate chemical properties, making it the most suitable candidate for chemical dominated combustion like premixed engine combustion. Alternatively, S2 displayed outstanding spray-guided combustion behavior because of the stringent chemical and physical target properties assigned. It is worthwhile to note that this new method of formulating surrogates for different applications was efficient and time-saving. Finally, we aim to perform experimental validation tests for CN, density, viscosity, surface tension, TSI, sooting tendency and particle size distribution to further support the validity of the current proposed jet fuel surrogates (S1 and S2) in the future.

1. Introduction

As one of the most significant classes of fuel for transportation, jet fuel is being widely used in the aviation industry. In the civil industry, jet fuels such as Jet-A and Jet-A-1 were utilized for civil aviation, while in the military field, aircraft were usually fueled with JP-8 which is rather similar to Jet-A [1]. Apart from being used in the aviation field especially in gas turbines, jet fuel has also witnessed a growing demand in diesel engines for ground vehicles and generators. One of the most powerful driving forces is the fact that the usage of jet fuel in both gas turbines and diesel engines is following the Army's single fuel forward policy for the simplification of supply chain logistics [2]. Another reason that cannot be neglected is that the adulteration of diesel with jet fuel is very popular in some countries and regions of the world [3]. As a result, it is necessary to perform more research on the usage of jet

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fuel in diesel engines and to investigate the engine performance and emissions.

Both the real diesel or real jet fuel actually consists of hundreds of chemical species and to understand how these components affect the physical and chemical phenomenon such as spray and auto-ignition require a more reliable modeling approach as well as more compact surrogate chemical reaction mechanisms which are practical to be used for engine level computational fluid dynamics (CFD) applications. Therefore the surrogates must precisely emulate the target properties and auto-ignition behavior of the real jet fuel with a handful of selected components; meanwhile the targets for the formulation of surrogates will be altered depending on the intended application of the surrogates. When being applied to compression ignition diesel engines, the physical properties of liquid phase fuels such as density, viscosity and surface tension are critical for spray development which influences the air/fuel mixing as well as thermal and compositional gradients. The ignition behavior is normally quantified by the cetane number (CN) while the hydrogen-carbon (H/C) ratio and lower heating value (LHV) determine the energy input and heat released during the oxidation of the fuel, respectively [4].

Great efforts have been taken by researchers in formulating jet fuel surrogates, developing chemical mechanisms and running experiments for validation. In 2002, Violi et al. [5] proposed a jet fuel surrogate with six components coupled with a mechanism from Ranzi [6]. The validation of this jet fuel surrogate in a shock tube experiment done by Vasu et al. [7] showed that it could only capture the ignition delay times at temperatures above 1000 K, but large error was exhibited at lower temperature. In 2005, Daguat and Cathonnet [1] pointed out that many jet fuel surrogate mechanisms were only validated for species concentrations at low pressure conditions which are not real engine relevant conditions. Then in 2006, Dagaut et al. [8] reported a new mechanism of kerosene Jet-A1 with 3-components (n-decane/n-propylbenzene/n-propylcyclohexane) that performed successfully for simulating the experiments in a jet stirred reactor over the high temperature range 900-1300 K, and for variable equivalence ratio ($0.5 \leq \phi \leq 2$). Gokulakrishnan et al. [9] extended the mechanism of kerosene-type fuels into four components (n-decane/n-decene/n-propylcyclohexane/ npropylbenzene) for gas turbine combustion simulation, wherein good predictions were achieved against jet stirred reactor reactivity profiles, and plug-flow reactor species time-history profiles, while ignition delay times were not validated extensively. A so-called Aachen surrogate mechanism of jet fuel containing only two major components (n-decane/1,2,4 trimethylbenzene) was proposed by Honnet et al. [10] in 2009, and produced good results in the critical conditions for auto-ignition of jet fuel. In 2010, Dooley et al. [11] proposed a method of formulating a specific jet fuel surrogate by empirical correlation of fuel properties, thus developing a jet fuel surrogate (1st generation, MURI1) composed of tri-component species (n-decane/iso-octane/toluene), which captured CN and H/C ratio of target jet fuel. Using such chemical kinetic model, produced new insight into the experimental observations and provided a rationale as to why the real jet fuel and surrogate fuel exhibit such similar reactivity. Later the second generation of the jet fuel surrogate MURI2 was created with four components (n-dodecane/iso-octane/n-propylbenzen/1,3,5-trimethylbenzene) also by Dooley et al. [12]. More physical properties of target jet fuel such as molecular weight (MW) and TSI were considered when formulating the jet fuel surrogate and the auto-ignition characteristics of this surrogate were verified by experiments in a shock tube at high pressures in both fuel lean and rich conditions [13]. Recently, two model-based surrogates of jet fuel UM1 (n-dodecane/iso-cetane/methylcyclohexane/toluene) and UM2 (n-dodecane/iso-cetane/decalin/toluene) were designed by Kim et al. [4] to emulate the chemical and physical properties of real jet fuel. UM1 was better to match for temperature-dependent properties while UM2 gave good results in liquid density and volatility. With detailed chemical mechanism that available in the literature, the ignition delay times predicted by these surrogate compositions showed reasonable agreement with the experimental data in shock tube studies.

Based on the comprehensive review above, although quite a number of jet fuel surrogates were developed to mimic the auto-ignition characteristics, some research gaps still exists: First, there is no jet fuel surrogate that can comprehensively reproduce the physical, gas phase chemical properties and sooting tendency of the target jet fuel. Secondly, the existing jet fuel surrogate mechanisms are quite few, while most of them are detailed mechanisms which currently are not practical to be utilized in the engine combustion CFD studies due to large mechanism size. Finally, few jet fuel surrogate detailed mechanisms have been comprehensively validated against ignition characteristics, species concentration profiles and laminar flame speed, not to mention a comprehensive validation for a skeletal mechanism.

As such, this study aims to design a jet fuel surrogate that is capable of emulating both chemical and physical properties along with sooting tendency under engine relevant conditions. Meanwhile, for engine application, the compositions in the surrogate fuel should include the major components of target real fuel and inherently satisfy the spray related physical characteristics and gas phase chemical properties as well as sooting index. Instead of tuning manually and empirically, an intelligent optimizer is introduced to facilitate the surrogate compositions precisely and economically while fulfilling the target properties. Moreover, in order to be coupled into engine level CFD study, the size of the chemical mechanisms of the surrogates should be concise and compact, and this is achieved by using the methodology of describing the chemistries for the oxidation of large molecules C_4–C_n and small molecules H_2/CO/C_1. Eventually, the performance of jet fuel surrogate and its associated skeletal mechanism are assessed by systematic validation against test data available in literature as follows: (1) accurate and comprehensive emulations for physical and chemical properties as well as TSI value of the target jet fuel, (2) validations against the experimental data of ignition delay times and species concentrations in shock tubes, jet stirred reactors and laminar premixed flames as well as laminar flame speed under a wide range of conditions, (3) 3-D validations for spray characteristic in a constant volume chamber. According to the demand of engine relevant combustion mode, two types of surrogates are formulated with the same components but different percentages hence leading to varied properties. In the present study, the candidate surrogate of jet fuel is individually proposed for homogenous dominated combustion mode like premixed engine combustion and spray-guided combustion.

2. Surrogate formulation

2.1. Surrogate target properties

The diesel engine combustion process is quite complex and normally can be divided into several distinctive periods, such as the ignition delay period, the premixed combustion period, the diffusion combustion period and the late combustion period [14]. The ignition delay time is strongly dependent on a number of physical and chemical processes when the liquid fuel is injected into the combustion chamber [15]. According to Reitz et al. [16,17], after the liquid fuel is injected, tiny liquid droplets will be generated due to the liquid fuel breaking up, which is inherently controlled by the ambient pressure, injection momentum along with the liquid fuel physical properties, such as density and viscosity. The subsequent