Fuel 181 (2016) 926–934

Contents lists available at ScienceDirect

Fuel

journal homepage: www.elsevier.com/locate/fuel

Full Length Article

Development of a reduced kerosene–diesel reaction mechanism with embedded soot chemistry for diesel engines

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HIGHLIGHTS

- The mechanism predicts the shock tube ignition delay times of Jet-A/JP-8 well.
- JP-8 ignition delay times are well predicted in a constant volume combustion chamber.
- Kerosene and diesel soot trends are well predicted in engine simulations.

ARTICLE INFO

Article history:
Received 15 January 2016
Received in revised form 29 March 2016
Accepted 4 May 2016
Available online 11 May 2016

Keywords:
Kerosene
Diesel
Reaction mechanism
Constant volume combustion chamber
Diesel engine

ABSTRACT

Kerosene combustion in diesel engines is getting more prevalent due to the push for kerosene use in diesel engines by the North Atlantic Treaty Organization military. The study of kerosene combustion in diesel engines has primarily been carried out through engine experiments. Negligible study has been carried out through engine simulations possibly due to the lack of a compact and reliable kerosene reaction mechanism. A compact and well validated kerosene reaction mechanism with embedded soot chemistry for diesel engine simulations is still lacking. In this work, a kerosene–diesel reaction mechanism, containing only 123 species and 586 reactions, is developed. Diesel is represented by $C_{14}H_{28}$ while kerosene is represented by $C_{12}H_{24}$. Both $C_{14}H_{28}$ and $C_{12}H_{24}$ are assumed to be oxidized via global reaction steps. The kerosene sub-mechanism is well validated for its ignition delay times under different initial shock tube conditions of 20 atm at equivalence ratios of 0.25, 0.5, 1.0, 1.5 and 2.0 for temperatures between 700 and 1400 K. Moreover, constant volume combustion validations were carried out under ambient conditions of 900 K/6.0 MPa and 1000 K/6.7 MPa. It is seen that the newly developed mechanism is able to closely replicate the heat-release rates and flame lift-off lengths under these ambient conditions. In addition, constant volume ignition delay validations were done under ambient densities of 14.8 kg/m^3 and 30.0 kg/m^3 for temperatures between 800 and 1250 K. The simulated and experimental constant volume ignition delays are very similar. Furthermore, the reaction mechanism is able to predict the combustion characteristics and soot trends of kerosene and diesel well under real engine conditions. In all, this newly developed kerosene–diesel reaction mechanism is suitable to be used for diesel engine simulations.

1. Introduction

Of the many alternative fuels such as gasoline [1] and biodiesel [2], it has been noted that the use of kerosene in diesel engines is getting more prevalent [3] and this is due to two main reasons. Firstly, the North Atlantic treaty Organization (NATO) military is encouraging the use of Jet Propellant 8 (JP-8) in all their engines, including diesel engines [4]. This is in line with their Single Fuel Concept (SFC) [4]. Secondly, in some countries, fuel adulteration [5] is a serious issue whereby kerosene is illegally mixed with diesel. With this in view, it is highly desirable to study the performance and emissions of kerosene and its blends in diesel engines. Although experimental studies have been carried out for kerosene combustion in diesel engines such as in [3], the poor lubricity property of kerosene [6] makes it impractical to run high ratios of kerosene blends in diesel engines as repeated running will cause engine damage. Moreover, numerical simulations of engine combustion will enable a better understanding of the combustion and emission characteristics of a particular fuel as highlighted by Li et al. [1].

Currently, there are many reaction mechanisms available in literature for various fuels such as gasoline [7], diesel [8], biodiesel [9] and their blends [10]. Those mechanisms are mainly tailored

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http://dx.doi.org/10.1016/j.fuel.2016.05.029
0016-2361/

to be used for compression ignition engines. Although there are quite a number of reaction mechanisms available for kerosene combustion, they are mainly tailored to be used under gas turbine engine conditions such as in [11,12]. From the review of Dagaut and Cathonnet [13], it is seen that many of the reaction mechanisms representing kerosene combustion are comprised of components such as n-decane, n-dodecane, toluene, n-propylbenzene and n-propylcyclohexane. Many of the reaction mechanisms were predominantly validated for their species concentration under jet-stirred reactors (JSRs) and premixed flame burners, with little to no validation for their ignition delay times against that of kerosene shock tube experiments. Also, some of the mechanisms are quite big in size. Next, Dagaut et al. [12] went on to propose kerosene surrogates using different combinations of n-decane, n-propylbenzene and n-propylcyclohexane. Initially, four combinations were proposed and they were n-decane, n-decane/n-propylcyclohexane, n-decane/n-propylbenzene and n-decane/n-propylbenzene/n-propylcyclohexane. Of the four combinations, it is observed that the three-component kerosene surrogate, containing n-decane/n-propylbenzene/n-propylcyclohexane in mole fractions of 0.74/0.15/0.11, gave the best speciation profiles under JSR and premixed flame conditions. However, ignition delay times of the three-component surrogate were not validated against kerosene shock tube experiments. Furthermore, Gokulakrishnan et al. [11] went on to develop a kerosene surrogate reaction mechanism consisting of about 550 species amongst 1400 reactions. The mechanism comprised of four carefully selected components, namely n-decane, n-propylcyclohexane, n-propylbenzene and decene, to represent the main classes of compounds in real kerosene. This mechanism was validated for its speciation data against JP-8 in a flow reactor and Jet A-1 in a JSR. The ignition delay times of the mechanism were validated against that of kerosene Jet-A experiments, but the range of validated conditions was rather limited. Also, Honnet et al. [14] developed a kerosene surrogate reaction mechanism consisting of 122 species amongst 900 reactions, known as the Aachen surrogate. The mechanism comprised of two components which are n-decane and 1,2,4-trimethylbenzene. The ignition delay times of the n-decane component were validated against n-decane shock tube experiments and the mechanism was able to reasonably reproduce the laminar flame speeds and soot volume fraction of real kerosene. More recent notable work was done by Dooley et al. [15] whereby they proposed a detailed kerosene surrogate mechanism consisting of n-decane/iso-octane/toluene, with 1599 species amongst 6633 reactions. The n-decane/iso-octane/toluene mixture is in the mole ratio of 0.4267/0.3302/0.2431 and it satisfied the derived cetane number (DCN) and hydrogen-to-carbon (H/C) ratio criteria. Moreover, this three component mechanism was able to reproduce the speciation data of kerosene in a flow reactor reasonably well. Notably, Cung et al. [16] used this mechanism in their study of soot formation of kerosene under diesel engine conditions. Building on Dooley et al.'s [15] mechanism, Malewicki et al. [17] developed a four component kerosene surrogate mechanism consisting of n-dodecane/iso-octane/n-propylbenzene/1,3,5-trimethylbenzene with a mole fraction of 40.4/29.5/22.8/7.3. This detailed four component mechanism consisted of 2080 species and 8310 reactions. The four components were carefully chosen to fulfil certain constrains which were important in the development of surrogate fuels that can imitate real fuels [18]. Hence, to imitate kerosene, a mixture of n-dodecane/iso-octane/n-propylbenzene/1,3,5-trimethylbenzene was chosen in a certain proportion to satisfy four constrains which were the molecular weight (MW), threshold sooting index (TSI), DCN and H/C ratio [18]. Refer to [18] for more details. Malewicki et al.'s [17] mechanism was able to reproduce the speciation data in a shock tube and flow reactor reasonably well. Next, Kim et al. [19] went on to develop two kerosene surrogates that were able to emulate both the chemical and thermo-physical properties of kerosene. There were eight target properties used by Kim et al. [19] during surrogate formulation, of which three were chemical properties and they are CN, H/C ratio and lower heating value (LHV). The two surrogates were UM1 and UM2, consisting of 0.3844 n-dodecane/0.1484 iso-cetane/0.2336 methylcyclohexane/0.2336 toluene and 0.2897 n-dodecane/0.1424 iso-cetane/0.3188 decalin/0.2491 toluene by mole fraction respectively. It is seen that UM2 better emulates the density and viscosity of real kerosene. Although the sizes of UM1 and UM2 were not given, it is believed that both UM1 and UM2 are quite big. In addition to the above works, Tay et al. [20] went on to develop a robust and compact kerosene–diesel reaction mechanism specifically for diesel engines. The mechanism comprised of 48 species and 152 reactions and it was validated extensively with kerosene shock tube and constant volume combustion experiments. However, this mechanism lacked soot formation and oxidation reactions. Two other works were done regarding kerosene combustion reaction mechanism. Vandersickel et al. [21] used a global reaction mechanism approach that required only 8 species and 7 reactions to simulate the combustion chemistry of distillate fuels. However, it should be noted that using this strategy means that important reactions on poly-aromatic hydrocarbon (PAH), soot and nitrogen oxides (NO_x) formation will be neglected. The other work was done by Kavuri et al. [22] in which a combination of n-heptane and iso-octane were used to reproduce the CN of kerosene. However, no ignition delay validation was done against that of kerosene shock tube experiments. Refer to [21,22] for more details.

From the aforementioned works, it can be seen that most kerosene surrogate mechanisms' ignition delay times were not extensively validated against that of kerosene shock tube as well as constant volume combustion experiments. It should be noted that a fuel's ignition delay will affect both the performance and emissions of diesel engines [23] and so extensive validation of ignition delay times under different conditions is important. Furthermore, as some mechanisms are rather huge in size, it is not practical for them to be used in engine simulations as it will consume much computational time. More importantly, it is extremely desirable to have a mechanism that can predict soot trends in diesel engines for both kerosene and diesel fuels. Although some mechanisms such as [17,14] have PAH formation reactions, the total number of reactions is just too big to be used for engine simulations.

Therefore, the objective of this work is to develop a relatively small but comprehensive kerosene–diesel reaction mechanism for diesel engine simulations. The developed mechanism must be able to reasonably predict soot trends of kerosene and diesel combustion. Also, kerosene and diesel will be represented each by a single fuel component to keep the mechanism size small. Furthermore, to ensure the reliability and robustness of the mechanism, a series of vigorous validations will be carried out and they are (a) shock tube ignition delay validation, (b) flame lift-off length, heat-release and ignition delay validation in a constant volume combustion chamber and (c) optical engine validation. It should be noted at this point that the majority of this work will be much focused on the development of the kerosene sub-mechanism although some work will also be done on the diesel sub-mechanism.

2. Modelling methodology

It should be noted that distillate fuels such as kerosene and diesel contains aromatic compounds [24] which contribute to the formation of soot. To construct a mechanism with soot chemistry, PAH reactions are important as PAH formation will eventually lead to the development of soot like in [25,26]. Thus, the starting