Energy Conversion and Management 108 (2016) 446–458

Contents lists available at ScienceDirect

Energy Conversion and Management

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

Development of a robust and compact kerosene–diesel reaction mechanism for diesel engines

Kun Lin Tay, Wenming Yang *, Balaji Mohan, Hui An, Dezhi Zhou, Wenbin Yu

Department of Mechanical Engineering, Faculty of Engineering, National University of Singapore, 9 Engineering Drive 1, Singapore 117576, Singapore

ARTICLE INFO

Article history:
Received 17 August 2015
Accepted 7 November 2015

Keywords:
Kerosene
Jet-A
JP-8
Reaction mechanism
Constant volume combustion chamber
Diesel engine

ABSTRACT

The use of kerosene fuels in internal combustion engines is getting more widespread. The North Atlantic Treaty Organization military is pushing for the use of a single fuel on the battlefield in order to reduce logistical issues. Moreover, in some countries, fuel adulteration is a serious matter where kerosene is blended with diesel and used in diesel engines. So far, most investigations done regarding the use of kerosene fuels in diesel engines are experimental and there is negligible simulation work done in this area possibly because of the lack of a robust and compact kerosene reaction mechanism. This work focuses on the development of a small but reliable kerosene–diesel reaction mechanism, suitable to be used for diesel engine simulations. The new kerosene–diesel reaction mechanism consists only of 48 species and 152 reactions. Furthermore, the kerosene sub-mechanism in this new mechanism is well validated for its ignition delay times and has proven to replicate kerosene combustion well in a constant volume combustion chamber and an optical engine. Overall, this new kerosene–diesel reaction mechanism is proven to be robust and practical for diesel engine simulations.

1. Introduction

Kerosene is one important class of transportation fuel amongst many others such as gasoline, diesel and biodiesel. In general, kerosene is being primarily used in the aviation industry. In civil aviation, Jet-A and Jet A-1 are utilized while JP-8 is used for military aviation [1]. In essence, civilian and military aviation fuels are very similar in terms of chemical composition except for the additives employed [1]. Moreover, as seen from Vasu et al.'s [2] work, the ignition delay times of Jet-A and JP-8 are very similar.

Although kerosene is primarily used in the aviation sector particularly in gas turbine engines, it is also used in internal combustion engines like diesel engines. One of the greatest driving forces behind kerosene usage in diesel engines is the fact that the North Atlantic Treaty Organization (NATO) military is intending to use JP-8 for all their automobiles and equipments due to logistical benefits and this concept is termed as Single Fuel Concept (SFC) [3]. Secondly, fuel adulteration is a big problem in some parts of the world where diesel is adulterated with kerosene for use in vehicles [4]. Therefore, there is definitely a demand for more research to be done for kerosene-fueled diesel engines to study its advantages and shortcomings, as well as to optimize the engine performance fueled with kerosene under different operating conditions. Since there is negligible numerical simulation study for kerosene-fueled diesel engines in literature, it is desirable to develop a reaction mechanism for kerosene suitable for diesel engine simulations. This will enable researchers to better study the effects of kerosene in diesel engines especially where it is experimentally challenging or impractical. One classic example is the use of pure kerosene in diesel engines such as in [5], where too high a concentration of kerosene fuel may cause wear and tear to the fuel supply system [3].

The research community has been working hard to develop reaction mechanisms for kerosene. From a 2005 review paper written by Dagaut and Cathonnet [1], it can be seen that n-decane is one of the most popular choices used to represent kerosene fuels, either as a mixture with other compounds or by itself. Furthermore, it is also seen from this review paper that most surrogate mechanisms for kerosene fuels were validated for species concentration generally under lower pressure conditions as compared to diesel engine conditions, not exceeding 40 atm, in jet-stirred reactors (JSRs) and premixed flame burners. Moreover, Dagaut et al. [6] used four different surrogate mechanisms to simulate kerosene combustion. Of the four mechanisms, the 3-component surrogate mechanism consisting of 74% n-decane/15% n-propylbenzene/11% n-propylcyclohexane by mole fraction gave the best performance under JSR conditions. Next, Gokulakrishnan et al. [7] developed a detailed 4-component

* Corresponding author. Tel.: +65 6516 6481.
E-mail address: mpeywm@nus.edu.sg (W. Yang).

http://dx.doi.org/10.1016/j.enconman.2015.11.018
0196-8904/

mechanism containing an estimated 550 species amongst 1400 reactions for gas turbine applications. The 4-component model uses n-decane, n-decene, n-propylcyclohexane and n-propylbenzene to represent the main classes of organic compounds in kerosene. Using this approach, the speciation data for Jet A-1 was reasonably well reproduced under JSR conditions and the ignition delay times of Jet-A were rather well reproduced under some conditions. However, the validation of ignition delay times was not extensive. Furthermore, Honnet et al. [8] developed a kerosene surrogate mechanism containing 2 major components (80% n-decane/20% 1,2,4-trimethylbenzene by weight), which has 122 species amongst 900 reactions. Critical conditions of autoignition of kerosene were mimicked under laminar non-premixed flow conditions. In addition, Wang et al. [9] developed a reduced 3-component surrogate for kerosene combustion (74% n-decane/15% n-propylbenzene/11% n-propylcyclohexane by mole fraction) from the work of Dagaut et al. [1], resulting in a mechanism with 106 species amongst 382 reactions. High temperature ignition delay times above 1000 K were validated with that of the detailed mechanism and speciation profiles were also well validated with that of the detailed mechanism. Besides, Zeng et al. [10] developed a skeletal n-decane mechanism to represent kerosene in gas turbine applications, consisting of 50 species amongst 210 reactions. The mechanism was validated with n-decane shock tube experiments and laminar premixed flames.

From the works highlighted above, it is interesting to note that the number of species and reactions for some mechanisms are quite large and is not practical for 3-dimensional (3-D) engine simulations. Furthermore, it can be seen that most works had only validated their mechanisms' species concentration during oxidation, with little validation done for ignition delay times. Hence, those mechanisms are not sufficiently validated to be used in diesel engines as diesel engines' performance depend very much on the ignition delay times of the fuel [11]. In addition, as observed previously, n-decane is a popular representative for kerosene. However, from Fig. 1, which shows the shock tube ignition delay times comparison between Chang et al.'s [12] n-decane mechanism and that of Jet-A/JP-8 experimental data [2,13–16] at 20 atm and 1.0 equivalence ratio; it is seen that the ignition delay times of n-decane and Jet-A/JP-8 fuels are quite different both in the high and low temperature regions. So, it can be concluded that n-decane has its limitations to be used as a kerosene surrogate under diesel engine conditions.

More recent notable works on kerosene modelling were done by Dooley et al. [16], Malewicki et al. [17] and Kim et al. [18]. Dooley et al.'s [16] 1st generation MURI[1] Jet-A surrogate have three fuel components (0.4267 n-decane/0.3302 iso-octane/0.2431 toluene by mole fraction) and contains 1599 species amongst 6633 reactions while that of Malewicki et al.'s [17] 2nd generation MURI Jet-A surrogate have four fuel components (0.404 n-dodecane/0.295 iso-octane/0.228 n-propylbenzene/0.073 1,3,5-trimethylbenzene by mole fraction) and contains 2080 species amongst 8310 reactions. Furthermore, although the number of species and reactions are unavailable for Kim et al.'s [18] UM1 (n-dodecane/iso-cetane/methyl cyclohexane/toluene) and UM2 (n-dodecane/iso-cetane/decalin/tol uene) Jet-A surrogates, it is believed that the size of UM1 and UM2 are comparable to that of MURI's Jet-A surrogate mechanisms as both UM1 and UM2 are also four-component surrogates. Because of the huge mechanism sizes, incorporating these large mechanisms for 3-D engine simulations is not practical as much more computational time is required. Interestingly, Dooley et al.'s [16] mechanism was used by Cung et al. [20] to model JP-8 combustion under diesel engine conditions.

[1] MURI stands for Multidisciplinary University Research Initiative [19] Multidisciplinary University Research Initiative (MURI). 2012. http://www.arl.army.mil/www/default.cfm?page=472.

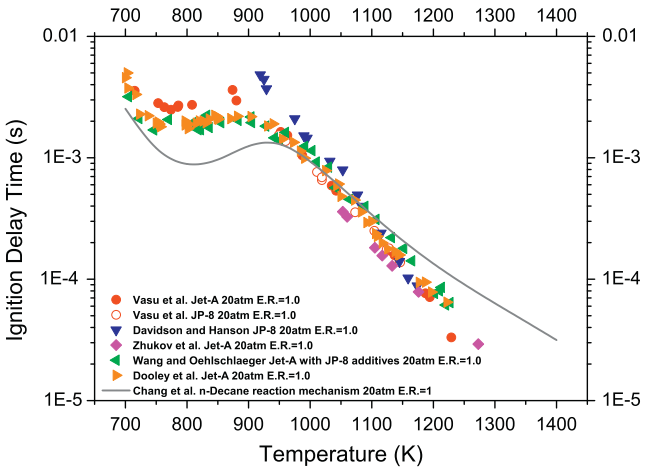

Fig. 1. Comparison of ignition delay times of n-decane (from Chang et al.'s reaction mechanism) and Jet-A/JP-8 experimental shock tube results (from Vasu et al. [2], Davidson and Hanson [13], Zhukov et al. [14], Wang and Oehlschlaeger [15] and Dooley et al. [16]) for initial shock tube conditions of 20 atm and 1.0 equivalence ratio.

Another interesting work was done by Vandersickel et al. [21] in which they used a global reaction mechanism approach to model the combustion of a complex class of fuel such as gasoline or kerosene. Using this method, the number of species and reactions are kept very low, with only 7 reactions and 8 species. It is proven in their paper [21] that this method is able to accurately reproduce the combustion of a complex class of fuel under homogeneous charge compression ignition (HCCI) conditions. However, it should be noted that no validation is done under non-HCCI conditions.

Moving on, from the work of Kavuri et al. [22], in which they investigated the impact on engine emissions when fuels with different cetane values are used, they employed a combination of n-heptane and iso-octane to represent kerosene. Although the cetane value of the 2-component kerosene surrogate is the same as that of real kerosene [22], the ignition delay times of the kerosene surrogate were not validated with that of kerosene shock tube experiments.

From the above comprehensive review, it is desirable to develop an accurate and compact surrogate mechanism for kerosene–diesel combustion in diesel engines as many kerosene mechanisms from literature are large and are designed for gas turbine conditions. Therefore, the objective of this work is to develop a reliable and compact reaction mechanism for kerosene–diesel combustion under diesel engine conditions, with an extra focus on the kerosene sub-mechanism. Kerosene will only be represented by a single component to allow for a more compact kerosene–diesel mechanism. The newly developed kerosene sub-mechanism must be able to imitate the heat-release characteristic and ignition delay times of real kerosene. As this work only focuses on replicating the heat-release and ignition delay times of real kerosene, polyaromatic hydrocarbon (PAH) and soot formation will not be included. To ensure the fidelity of this new mechanism, especially for the kerosene sub-mechanism, a systematic validation will be performed: (a) 0-D shock tube ignition delay validation, (b) 3-D constant volume heat-release rate, OH profile and ignition delay validation and (c) 3-D engine validation.

2. Chemical modelling

In order to develop a kerosene–diesel reaction mechanism, a suitable reaction mechanism representing diesel has to be first selected. The diesel chemistry is usually represented simply by n-heptane and there are numerous reaction mechanisms available in literature for n-heptane, both skeletal [23] and detailed [24].