



# Development of a new skeletal mechanism for n-decane oxidation under engine-relevant conditions based on a decoupling methodology



Yachao Chang, Ming Jia<sup>\*</sup>, Yaodong Liu, Yaopeng Li, Maozhao Xie

Key Laboratory of Ocean Energy Utilization and Energy Conservation of Ministry of Education, School of Energy and Power Engineering, Dalian University of Technology, PR China

## ARTICLE INFO

### Article history:

Received 14 November 2012  
 Received in revised form 16 February 2013  
 Accepted 19 February 2013  
 Available online 13 March 2013

### Keywords:

n-Decane oxidation  
 Skeletal mechanism  
 Decoupling methodology  
 Internal combustion engine

## ABSTRACT

A new skeletal mechanism for n-decane oxidation was developed based on a decoupling methodology with the special emphasis on the engine-relevant operating conditions from low to high temperature at high pressure. With the decoupling methodology, an extremely simplified model for C<sub>2</sub>–C<sub>10</sub> was used to simulate the oxidation of heavy hydrocarbons for prediction of the ignition characteristics, while the mechanism of H<sub>2</sub>/CO/C<sub>1</sub> was considered in details for providing accurate information of laminar flame speed and extinction strain rate. The new skeletal n-decane oxidation mechanism consists of 40 species and 141 reactions. Extensive validations of the present mechanism were performed by comparing with the experimental data available in the literature on n-decane oxidation, including ignition delay in shock tube and rapid compression machine, species concentrations in jet-stirred reactor and variable pressure flow reactor in wide ranges of temperature (550–1800 K), pressure (1–80 bar) and equivalence ratio (0.5–2). Moreover, the experimental data on the profiles of species concentration, laminar flame speed and extinction strain rate in premixed flame and counterflow flame was also being used in the validations. Finally, the skeletal n-decane mechanism was applied to predict the combustion and emissions of premixed charge compression ignition (PCCI) engines by using the multi-dimensional simulation. Overall, the current prediction from the present mechanism shows a good agreement with the experimental measurements, which indicates the potential of the decoupling methodology for the development of oxidation mechanism for heavy alkanes.

© 2013 The Combustion Institute. Published by Elsevier Inc. All rights reserved.

## 1. Introduction

With the global energy crisis and stringent emission legislation, diesel engine is under great pressure for further improvement of fuel economy and reduction of emissions. The new combustion strategies including homogeneous charge compression ignition (HCCI), premixed charge compression ignition (PCCI) and reactivity controlled compression ignition (RCCI) have attracted increasing attentions in the recent years, because they can provide very low nitrogen oxides (NO<sub>x</sub>) and particulate matter (PM) emissions while maintaining the high fuel efficiency for diesel engines [1–3]. It was highlighted by Westbrook et al. [4] that computational combustion is a major contributing factor for the growth of HCCI from an idea to reality in a very short time. Because chemical kinetics of fuel plays a dominant role in the combustion process of HCCI, PCCI and RCCI engines, it is extremely crucial to construct a robust chemical kinetic model for engine simulation.

The commercial diesel fuel consists of hundreds of species, and the complexity of fuel prevents the development of a detailed mechanism to describe the oxidation and combustion of diesel fuel. Thus, the simplified surrogate fuel is usually used to represent the real diesel. A surrogate fuel is defined as a fuel composed of a small number of pure compounds whose behavior matches certain characteristics of a target fuel that contains many compounds [5,6]. Normal-decane (n-decane) has been considered as a major surrogate component for diesel fuel [7–13]. By reviewing the progress of diesel surrogate fuel, Farrell et al. [6] recommended the near-term diesel surrogate should be comprised of n-decane, iso-octane, methylcyclohexane, and/or toluene.

Several n-decane oxidation mechanisms have been developed in recent decades. By organizing a large number of elementary reactions into 25 reaction classes, Westbrook et al. [14] developed a detailed mechanism to describe the pyrolysis and oxidation from n-octane to n-hexadecane. For n-decane, the mechanism includes 940 species and 3878 elementary reactions, and the mechanism was compared with the experimental data including shock tube, rapid compression machine (RCM), flow reactor and jet-stirred reactor (JSR) under wide ranges of temperature, pressure and equivalence ratio. The mechanism prediction shows a good

<sup>\*</sup> Corresponding author. Address: School of Energy and Power Engineering, Dalian University of Technology, Dalian 116024, PR China. Fax: +86 411 84706302.  
 E-mail address: [jjaming@dlut.edu.cn](mailto:jjaming@dlut.edu.cn) (M. Jia).

agreement with the experimental results at most conditions. However, for high pressure shock tube ignition, the model predicted a longer ignition delay time by a factor of two. More recently, a detailed chemical kinetic mechanism has been developed by Titova et al. [15] to study the pyrolysis and oxidation of n-decane in shock tube and flow reactor. The elementary reactions are organized into 22 reaction classes which are common used to describe the oxidation of n-alkanes.

The detailed mechanism for n-decane oxidation includes thousands of reactions. Especially at low temperature, a large number of intermediate species are involved. Therefore, it is difficult to construct a detailed mechanism manually. Several computer programs have been developed to automatically generate the mechanism for n-decane oxidation automatically, such as EXGAS [16–20], LISP [21], MOLEC [22] and MAMOX++ [23]. The detailed mechanisms generated by the automatic programs include both the low- and high-temperature mechanisms, and usually consist of hundreds of species and thousands of elementary reactions. Thus, the ignition delay time in shock tube and the mole fraction profiles of species in jet-stirred reactor can be reasonably predicted by these detailed mechanisms.

However, the size of detailed mechanism prevents its use in multidimensional simulation of engine combustion. To solve the problem, many researchers [24–29] tried to build the reduced and skeletal mechanisms. Zeppieri et al. [24] developed a partially reduced skeletal mechanism for the pyrolysis and oxidation of n-decane by using the assumption that the n-alkyl radicals with more than four carbon atoms is in isometric partial equilibrium. Whereas the mechanism for species with carbon number fewer than four was simulated with detailed elementary kinetics. The model developed by Zeppieri et al. [24] reproduced the experimental data well in flow reactor, jet-stirred reactor and shock tube data under high-temperature conditions. Zhao et al. [25] improved the model of Zeppieri et al. [24] by updating the  $C_1$ – $C_3$  sub-mechanism in order to better predict the premixed laminar flame speed.

It should be noted that most of skeletal mechanisms consider only the high-temperature reactions currently. By lumping the low-temperature reactions, Bikas and Peters [26] developed a semi-detailed n-decane mechanism including 67 species and 600 elementary reactions. The mechanism can be used to describe the oxidation of n-decane from low temperature to high temperature with validations in shock tube, jet-stirred reactor, and premixed laminar flame. More recently, Honnet et al. [30] modified the n-decane model of Bikas and Peters [26] in order to improve the agreement with ignition delay at low temperature in shock tube.

In this paper, a new skeletal mechanism was developed to describe the oxidation of n-decane for multi-dimensional simulation of advanced diesel engines. The first purpose of this work is to construct a reliable and accurate n-decane oxidation model for engine-relevant conditions with special emphasis on the combustion and emission characteristics including ignition delay at low- and intermediate temperatures, heat release rate, species concentrations of small hydrocarbon (HC), carbon monoxide (CO) and  $NO_x$ , as well as the laminar flame speed and extinction strain rate under high-pressure conditions. The validation of acetylene evolution is also considered because acetylene has been treated as the most relevant species for soot formation in hydrocarbon fuels. The second purpose of this work is to explore how simple the n-decane oxidation model could be. In order to satisfy the requirement of the model for engine multi-dimensional simulation and minimize the number of species, a decoupling methodology by integrating the skeletal mechanism for  $C_2$ – $C_{10}$  with the detailed sub-mechanism for  $H_2/CO/C_1$  was proposed.

## 2. Model development

As mentioned above, the detailed mechanism of n-decane oxidation usually consists of hundreds of species and thousands of reactions. Thus, it needs a huge amount of computational power to apply such detailed mechanism to multi-dimensional simulations of engine combustion. To solve this problem, various mechanism reduction methods have been developed for the simplification of the detailed model. It should be noted that the accuracy of the detailed mechanism will lose to some extent with the global reduction of the detailed mechanism under wide engine operating ranges. In addition, it has been found by Sun et al. [31] that the reduced n-decane mechanism generated from a detailed mechanism (116 species) by the reduction methods of path flux analysis and direct relation graph (DRG) have 54 and 55 species, respectively, which reaches the limit of these methods. Because the computational time exponentially increases with the number of species, further reduction of the size of the kinetic mechanism is still pursued.

A decoupling methodology was proposed in this study, which is an extension of our previous work for n-heptane and iso-octane models [32,33]. In the decoupling methodology, the chemistries for the oxidation of small molecules  $H_2/CO/C_1$  and larger ones  $C_2$ – $C_{10}$  were described separately. An extremely simplified model for  $C_2$ – $C_{10}$  was used to model the oxidation of heavy hydrocarbons, while the mechanism of  $H_2/CO/C_1$  was considered in details. By applying a well-established simplified auto-ignition model for the oxidation of heavy hydrocarbons [34–36], only the representative species were retained to predict the ignition delay of the n-decane. The simplification of the mechanism for  $C_2$ – $C_{10}$  dramatically decreases the number of species in the final n-decane oxidation model. The two sub-mechanisms for  $H_2/CO/C_1$  and  $C_2$ – $C_{10}$  were integrated by introducing the reactions for direct decomposition of the intermediate species with carbon number higher than two into  $H_2/CO/C_1$  species.

The detailed mechanism of  $H_2/CO/C_1$  is employed in this study is due to the following four reasons. Firstly, it has been widely accepted that the laminar flame speed of heavy n-alkanes is dominated by the oxidation kinetics of small radical and molecular species, especially hydrogen radical and methyl radical [37]. Meanwhile, Ji et al. [38] found that the extinction strain rate of  $C_5$ – $C_{12}$  n-alkane is mostly sensitive to  $H_2/CO/C_1$ – $C_2$  kinetics and not to fuel-specific reactions. Secondly, the important species for engine modeling, such as small hydrocarbons and CO should be described in details in order to provide accurate predictions for the related emissions. Thirdly, it was indicated that most of the heat release is from the oxidation reaction of CO to  $CO_2$  for the oxidation of heavy hydrocarbons [39], so the detailed mechanism for CO oxidation is necessary for the prediction of the heat release processes of engine combustion, which further determines the evolution of in-cylinder temperature, and subsequently the  $NO_x$  emissions. Finally, the mechanism for  $H_2/CO/C_1$  has been well established compared to those for heavy hydrocarbons, and only a limited number of species is involved. Therefore, with the detailed mechanism for  $H_2/CO/C_1$ , a satisfactory prediction of heat release rate, laminar flame speed, extinction strain rate and emission characteristics can be achieved without significant increase of the species number in the final mechanism.

Overall, the decoupling methodology for development of n-decane oxidation mechanism has several advantages. Firstly, the application of detailed mechanism for  $H_2/CO/C_1$  in the n-decane model provides accurate predictions for laminar flame speed, extinction strain rate, heat release rate, as well as the emissions of small hydrocarbons and CO under wide ranges of temperature, pressure and equivalence ratio as aforementioned. Since the

Download English Version:

<https://daneshyari.com/en/article/168877>

Download Persian Version:

<https://daneshyari.com/article/168877>

[Daneshyari.com](https://daneshyari.com)