



Reduced kinetic mechanisms of diesel fuel surrogate for engine CFD simulations



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ARTICLE INFO

Article history:

Received 19 March 2015

Revised 27 July 2015

Accepted 28 July 2015

Available online 19 August 2015

Keywords:

n-Dodecane

Skeletal kinetic mechanism

Autoignition

Flame lift-off

Diesel spray combustion

ABSTRACT

Detailed chemistry represents a fundamental pre-requisite for a realistic simulation of combustion process in diesel engines. In this work, the authors developed a reduced mechanism for n-dodecane starting from the comprehensive POLIMI_TOT_1407 kinetic mechanism, already well validated and tested in a wide range of operating conditions. This reduced mechanism (96 species and 993 reactions) is able to accurately describe the high and low-temperature reactivity of n-dodecane in a wide range of conditions. This kinetic scheme has been extended to soot precursors by adding a relatively small sub-mechanism (37 species and 1282 reactions).

This work extensively validates this reduced kinetic scheme, together with similar skeletal mechanisms from the literature, using experimental data in a wide range of conditions, including flow and stirred reactors experiments, autoignition delay times, laminar flame speeds, and autoignition of isolated fuel droplets in microgravity conditions.

These kinetic mechanisms were then applied to diesel spray combustion modeling. The simulations were performed by using the MRIF (Multiple Representative Interactive Flamelets) model implemented in the Lib-ICE code. Comparisons to measured flame-lift off and ignition delays of the ECN (Engine Combustion Network) database at different operating conditions are discussed.

Even if all the kinetic mechanisms reasonably describe the ignition and combustion in ideal reactors and laminar flames and capture the important characteristics of spray ignition processes, relevant differences exist and are discussed in this work.

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1. Introduction

Diesel engines will remain for several decades one of the most important powertrain technologies for transportation [1,2]. However, to fulfill the requirements in terms of pollutant reduction and efficiency increase, different solutions are investigated, such as new combustion strategies and alternative fuels. Within this context, detailed numerical tools and reliable kinetic modeling of combustion are required [2], for a proper prediction of engine efficiency and pollutants (PAH, soot, NO_x, etc.). The description of the combustion process for the liquid fuels employed in transportations is a very complex task for two different reasons: the challenging characterization of the complex mixture of several hydrocarbon isomers, and the complexity of the oxidation mechanisms of large hydrocarbon and oxygenated molecules [3]. While surrogate mixtures of reference

components allow to tackle the first difficulty [4,5], the complex behavior of the oxidation mechanisms is mostly overcome by adopting a lumping approach [6,7].

Multi-dimensional simulations are now widely employed to design and develop direct-injection diesel engines. Most of the attention is focused on the combustion phase, due to the need to reduce pollutant emissions and increase thermal efficiency. To this aim, both standard and advanced combustion modes are widely studied, analyzing how fuel distribution and flame structure are affected by injection strategy, fuel composition, mixture, and thermal stratification [8–12]. However, the use of multiple injections and engine operation under advanced combustion modes involves a large variety of combustion regimes where fuel auto-ignition and flame propagation take place in a wide range of pressures, temperatures, and equivalence ratio conditions. Hence, realistic results can be achieved only if both complex fuel chemistry and its interaction with turbulence are properly taken into account inside a Computational Fluid Dynamics (CFD) simulation. These reasons justify the interest towards the development of skeletal kinetic models, especially considering that the

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computational cost scales by the second/third power of the number of species and that the very large sizes of detailed kinetic schemes could pose problems even in 1-D modeling [13].

Due to the similarity between $nC_{12}H_{26}$ and diesel fuel in terms of liquid and chemical properties, several spray combustion experiments were carried out in the SANDIA constant-volume vessel by using neat n-dodecane at different oxygen concentration. These data are publicly available through the Engine Combustion Network (www.ca.sandia.gov/ecn). All these reasons explain the interest towards the development of a skeletal kinetic model of n-dodecane oxidation.

In the following, different skeletal n-dodecane kinetic mechanisms are first investigated in ideal reactors, where reactivity is controlled only by chemical kinetics, in order to understand their characteristics, peculiarities and reliability in different operating conditions. These mechanisms are then further validated in comparison to measurements of 1D laminar flames and isolated fuel droplets in micro-gravity conditions, where diffusion also plays an important role. All these comparisons allow to better discuss the differences observed when these mechanisms are adopted in the modeling of more complex systems, where the use of CFD codes prevents detailed chemical analyses. Finally, paragraph 5 compares the predictions of these kinetic schemes in diesel-like spray conditions, using an unsteady flamelet based approach to model the turbulent non-premixed flame. Alternative and more complex turbulent combustion models could be adopted with the proposed skeletal kinetic mechanism, but their comparison is out of the scopes of the present investigation.

2. Mechanism reduction: skeletal mechanism of n-dodecane oxidation

The kinetic modeling of the autoignition of hydrocarbon fuels in typical engine conditions requires a careful analysis of both low and high-temperature mechanisms. A general detailed kinetic scheme (POLIMI_TOT_1407) (<http://creckmodeling.chem.polimi.it/>), consisting of more than 450 species and ~15,000 reactions, was discussed in previous papers [6,14]. This comprehensive kinetic scheme is based on a detailed core mechanism of C1–C4-species, a lumped description of the primary propagation reactions of larger species and their primary intermediates, and permits description of the oxidation of hydrocarbons up to jet and diesel fuels, including also alcohols and biodiesel fuels [15]. This approach, together with an extensive use of structural analogies and similarities within the different reaction classes, easily allows extension of the scheme to new species [16].

This general kinetic model has been validated in a wide range of operating conditions through the comparison with experimental measurements carried out in well controlled reaction environments (jet stirred reactors, rapid compression machines, shock tubes, flow reactors, etc) [17–19], covering both high [15] and low temperature [6,14] conditions. The comprehensive validation proved the reliability of the mechanism in all the conditions relevant to engine combustion. The same kinetic scheme, which is also capable of simulating the combustion behavior of real transportation fuels [19,20], has been also successfully applied to the evaluation of the auto-ignition propensities of different fuel surrogate mixtures in SI and HCCI engines over a wide set of operating condition, as discussed in previous works [21–24].

Starting from this kinetic scheme (POLIMI_TOT_1407), a skeletal mechanism (Polimi_NC12_96) of n-dodecane combustion containing 96 species has been obtained using the approach previously described by Stagni et al. [7] and Ranzi et al. [19]. This reduced or skeletal kinetic scheme is discussed in the kinetic section of this paper and then used in the section of the spray engine modeling. The Supplemental material reports more details about the reduction procedure, the errors compared with the complete kinetic scheme, and the error maps (Fig. S1 in the SM) in the range of the validation conditions.

Table 1
n-dodecane skeletal mechanisms used in this work.

	Number of species	Number of reactions	Max error (%)	Original mechanism
Luo et al. [13]	105	420	30	[27]
Narayanaswamy et al. [25]	255	2289	18	[27]
Polimi_NC12_96	96	993	15	[Polimi
(extension to PAHs)	(133)	(2275)		TOT1407]
Wang et al. [26]	100	432	–	[28]

3. Validation of the skeletal model and comparison with similar literature mechanisms

This section contains an extensive validation study of the skeletal Polimi_NC12_96 kinetic mechanism in a very wide range of conditions, together with a similar validation and comparison with other n-dodecane skeletal mechanisms recently proposed in the literature. Table 1 compares the schemes of Narayanaswamy et al. [25], containing 255 species and 2289 reactions, the mechanism of Luo et al. [13] containing 105 species and 420 reactions, and the mechanism of Wang et al. [26] which has 100 species and 432 reactions. All these mechanisms were already validated and developed with accuracy targets similar to the ones adopted in this work. The mechanisms of Luo and Narayanaswamy were obtained from the detailed mechanism of Sarathy et al. [27], while the mechanism of Wang from the previous scheme of Westbrook et al. [28]. Luo et al. [13] adopted a combination of directed relation graph (DRG) [29] with expert knowledge (DRGX) [30] and DRG-aided sensitivity (DRGASA) [31] to obtain their skeletal mechanism. Narayanaswamy et al. [25] reduced the detailed scheme of Sarathy et al. [27] to a skeletal level using a multi-stage reduction strategy, involving automatic species and reaction elimination using the DRGEP approach [32], and chemical lumping of species [33]. Wang et al. [26] adopted a similar procedure based on the DRGEP method [32] with reaction pathway and sensitivity analyses to reduce the detailed mechanism of Westbrook et al. [28].

It is first useful to compare the structure of these mechanisms to highlight difference and similarities. Table 2 shows a comparison of the relevant species with 12 carbon atoms, formed in the low temperature oxidation of n-dodecane. The Luo mechanism maintains a small subset of the original isomers contained in the original detailed mechanism [27], while the other schemes also take advantage of the lumping approach to further reduce the number of species. Figure 1 shows the effect of the reduction on the number of species and their distribution in a C–H plane. It is possible to observe that the Luo mechanism only contains heavy species with high H/C ratios, i.e. the reduction phase eliminated all the heavy dehydrogenated and aromatic species. It is also evident that the mechanism still contains a relatively large number of species with 12 carbon atoms. The Wang mechanism has a similar structure, but takes advantage of the lumping approach and therefore it has only 5 species with 12 carbon atoms. As already observed in Table 2, Narayanaswamy et al. [25] partially used lumping rules to reduce the total number of isomers. This mechanism also contains heavy dehydrogenated species and PAHs leading to soot precursors, located in the region of the diagram corresponding to heavy species with low H/C ratios. The Polimi mechanism with 96 species has a similar structure, and thanks to the “horizontal lumping” approach it contains 6 species with 12 carbon atoms. This strategy is also combined to a “vertical lumping”: homologous species with 8, 9 and 11 carbon atoms are split between the two closest references (7, 10 or 12) according to the lever rule. Doing so, the total number of stable species is further reduced [6]. By adding a sub-set of 37 species and 1282 reactions, the mechanism can be extended to include benzene, indene, naphthalene, methyl-naphthalene, acenaphthylene, phenanthrene, biphenyl, fluorene and other aromatics up to C_{20} . Similarly, the scheme of Wang includes PAHs up to

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