Fuel 181 (2016) 120–130

Contents lists available at ScienceDirect

Fuel

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

Full Length Article

Development of multi-component diesel surrogate fuel models – Part II: Validation of the integrated mechanisms in 0-D kinetic and 2-D CFD spray combustion simulations

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HIGHLIGHTS

- 2 versions of multi-component diesel surrogate models were developed in this study.
- Surrogate models with different CN can be produced through blending of HXN and HMN.
- Inclusion of aromatics and cyclo-alkane components enhances soot predictions.
- MCDS1 serves as a potential surrogate model for diesel fuels with different CN.
- MCDS2 is a potential model for fuels with aromatics and cyclo-paraffinic contents.

ARTICLE INFO

Article history:
Received 16 December 2015
Received in revised form 4 March 2016
Accepted 22 April 2016
Available online 30 April 2016

Keywords:
Multi-component diesel surrogate
CFD simulations
Spray combustion
Chemical kinetic mechanism
Soot formation

ABSTRACT

The aim of this study is to develop compact yet comprehensive multi-component diesel surrogate fuel models for computational fluid dynamics (CFD) spray combustion modelling studies. The fuel constituent reduced mechanisms including n-hexadecane (HXN), 2,2,4,4,6,8,8-heptamethylnonane (HMN), cyclohexane (CHX) and toluene developed in Part I are applied in this work. They are combined to produce two different versions of multi-component diesel surrogate models in the form of MCDS1 (HXN + HMN) and MCDS2 (HXN + HMN + toluene + CHX). The integrated mechanisms are then comprehensively validated in zero-dimensional chemical kinetic simulations under a wide range of shock tube and jet stirred reactor conditions. Subsequently, the fidelity of the surrogate models is further evaluated in two-dimensional CFD spray combustion simulations. Simulation results show that ignition delay (ID) prediction corresponds well to the change of fuel constituent mass fraction which is calculated to match the cetane number (CN). In addition, comparisons of the simulation results to the experimental data of #2 diesel fuel (D2) in a constant volume combustion chamber show that IDs and lift-off lengths are reasonably well replicated by the models. The MCDS2 model is also found to perform better in the soot formation prediction in D2 fuel combustion as the model contains aromatic and cyclo-alkane components which provide an additional pathway to the formation of rich species such as C_2H_2 and C_6H_6. Implementation of MCDS2 predicts an increase of maximum local soot volume fraction by a factor of 2.1 when the ambient temperature increases from 900 K to 1000 K, while the prediction by MCDS1 is lower at 1.6. This trend qualitatively agrees with the experimental observation. This work demonstrates that MCDS1 serves as a potential surrogate fuel model for diesel fuels with CN values ranging from 15 to 100. It also shows that MCDS2 is a more appropriate surrogate model for fuels with aromatics and cyclo-paraffinic contents, particularly when soot calculation is of main interest.

1. Introduction

In multi-dimensional computational fluid dynamics (CFD) modelling studies [1–6], n-heptane has been widely utilised as a single-component diesel surrogate fuel model owing to its cetane number (CN) of 55, which is comparable to those of the actual

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http://dx.doi.org/10.1016/j.fuel.2016.04.114
0016-2361/

diesel fuels which range between 40 and 56 [7]. Nonetheless, actual diesel fuels generally consist of long carbon chain structure with 10–25 carbon atoms [7]. Fuels with long-chain n-alkanes exhibit higher reactivity at low temperatures as compared to those with short carbon chains. This is due to the higher ratio of secondary to primary hydrogen atoms which then increases the H-atom abstraction rate during the initiation phase of the oxidation of alkanes [8]. As a consequence, the combustion of long-chain hydrocarbons particularly n-hexadecane (HXN) [9] has become the centre of attention in many current research works [10–13]. HXN is the primary reference fuel and it has a CN of 100. Surrogate fuel models with different CN values can hence be produced when HXN is blended with other fuels such as 1-methylnaphthalene with a CN of 0 and 2,2,4,4,6,8,8-heptamethylnonane (HMN) with a CN of 15. Therefore, HXN has been identified as a promising component for diesel fuel surrogate model in recent works [12–14]. Nonetheless, it is evident that the Hydrogen/Carbon Molar Ratio (H/C) of HXN is different from that of the actual diesel fuels, on top of the difference in CN. H/C ratio is a key property in simulation studies in order to replicate combustion properties such as heat of reaction, local air/fuel stoichiometric location, flame temperature and flame speed [15]. It is important to note that similar restriction is expected to hold for any other single-component diesel surrogate fuels [16,17].

Apart from that, the Polycyclic Aromatic Hydrocarbons (PAH) formation in diesel fuel combustion is not well described by a single-component diesel surrogate fuel model [7]. In the experiment carried out by Kook and Pickett [18], soot formation of a surrogate fuel comprising 23% m-xylene and 77% n-dodecane (by volume) was studied and the sooting tendency was subsequently compared to a conventional jet fuel under diesel-engine like conditions. Their planar laser induced incandescence (PLII) measurement revealed that the soot level produced by the n-dodecane/m-xylene surrogate fuel is higher than that of the conventional jet fuel. For the combustion of fuels that do not contain aromatic compounds, the maximum local soot volume fraction (SVF) increases by a factor of approximately two when the ambient temperature rises from 900 K to 1000 K. On the other hand, the maximum SVF increases by a factor of at least five for the combustion of fuels which consist of aromatic volume of 23–27%. This corresponds with the reported experimental studies [19–22] where the sooting tendency of a single-component surrogate model is comparatively less significant than an alkane/aromatic mixture. Single component diesel surrogate models which do not contain PAH chemistry in its original fuel composition are hence debatable since actual diesel fuels contain 20–30% of aromatic compounds [23].

Recognizing the limitation of single-component diesel surrogate fuel models, development of surrogate models with matching fuel compositions as the actual diesel fuels is necessary. Consequently, multi-component diesel surrogate models with blends of various fuel components have been proposed [7,24–30]. The details of the surrogate mechanisms, together with their respective constitutional components are provided in Table 1. In the earlier years, the number of components in a surrogate model was limited owing to the complexity in solving the stiff ordinary differential equations and the associated high computational cost. Besides, huge quantity of work was required to develop the database and mechanistic understanding of the surrogate components for diesel fuels [7]. Fuel blends which are commonly employed in numerical simulations of diesel combustion are Integrated Diesel European Action (IDEA) mechanism [27,28,31], Primary Reference Fuels (PRF) mechanism [32–35] and Diesel Oil Surrogate (DOS) mechanism [36]. With rapid advancement in chemical kinetics as well as computing power, surrogate models with greater number of fuel components are established such as PRF+1 mechanism [24] and

Table 1
Details of the currently available multi-component surrogate fuel models.

Surrogate models	Compositions	N_S	N_R	Model descriptions	Year of Publication	Author(s)	Refs.
IDEA	n-decane, 1-methylnaphthalene	118	557	Describe fuel oxidation, soot and NOx formations; Contain low-temperature kinetics for auto-ignition	1999	Hergart et al.	[31]
PRF	iso-octane, n-heptane	990	4060	Describe auto-ignition and intermediate product formation at high-pressure conditions; Contain kinetic reactions for low to high temperatures as well as NTC behaviour	1998	Curran et al.	[32]
		58	120	Describe ignition of PRF in a HCCI engine; Contain kinetic reactions for intermediate and high temperatures	2007	Kirchen et al.	[33]
		73	296	Describe oxidation of diesel/gasoline; Contain kinetic reactions for low to high temperatures as	2013	Wang et al.	[34]
		1034	4236	well as NTC behaviour. Reduced model of Wang et al. [34] is developed based on the LLNL detailed model [35]	–	LLNL	[35]
Diesel PRF	HXN, HMN	2800	11,000	Contain alkylperoxy radical sub-mechanism and kinetic reactions for low to high temperatures as well as NTC behaviour	2011	Westbrook et al.	[26]
DOS	n-heptane, toluene	70	305	Describe fuel oxidation, soot and NOx formations; Optimised for engine applications	2007	Golovitchev et al.	[36]
PRF+1	iso-octane, n-heptane, toluene	469	1221	Describe fuel oxidation and soot formations; Contain kinetic reactions for low and intermediate temperatures	2007	Chaos et al.	[24]
TRF-PAH	n-heptane, toluene, PAH	71	360	Describe combustion and PAH formation; Contain kinetic reactions for low to high temperatures	2013	Wang et al.	[25]
POLIMI_Diesel_201	HXN, toluene, xylene, methylnaphthalene	201	4240	Validated under shock-tube (intermediate to high temperatures) and JSR (low to intermediate temperatures) simulations	2014	Ranzi et al.	[38]
POLIMI_NC12_96 + PAH	n-dodecane, PAH	133	2275	Contain kinetic reactions for low to high temperatures; Reasonably capture the important characteristics of spray ignition processes	2015	Frassoldati et al.	[30]
Skeletal Diesel Surrogate Fuel Model	n-decane, iso-octane, methylcyclohexane, toluene	70	220	Validated under shock-tube, JSR, flow reactor and pre-mixed laminar flame simulations	2015	Chang et al.	[29]

N_S and N_R denote the number of species and reactions, respectively; NTC is defined as negative temperature coefficient.