



Full Length Article

Development and validation of a reduced reaction mechanism with a focus on diesel fuel/syngas co-oxidation



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HIGHLIGHTS

- A reduced reaction mechanism for diesel/syngas RCCI engine combustion was developed.
- Chemistry interaction of multi-component fuels was considered in mechanism reduction.
- Conjugate-alkene and immediate lower level ketohydroperoxides should be retained.
- Reactions with OH/HO₂ have completing/assisting effects on co-oxidation.

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ABSTRACT

A reduced reaction mechanism has been developed for modeling Reactivity Controlled Compression Ignition (RCCI) engine combustion with diesel fuel and syngas. Employing *n*-heptane as a single representative chemical surrogate for diesel fuel, a comprehensive mechanism was reduced such that the reaction mechanism of syngas oxidation is included as a sub-mechanism with emphasis on the interaction of oxidation reaction pathways of syngas and *n*-heptane. Important reaction pathways to be kept in the reduced mechanism to maintain the performance of the detailed mechanism were identified through ignition delay curve sensitivity analysis. In addition, reaction steps to which ignition delays of multi-fuel blends are sensitive were identified and the importance of predictability of co-oxidation of multi-fuels in the mechanism reduction process was demonstrated.

The reduced mechanism, with 81 species and 312 reactions, was validated against experimental ignition delay times available in the literature. The reduced mechanism was also applied to simulate diesel-syngas RCCI engine combustion, employing a multi-component surrogate model to accurately model the physical properties of diesel fuel sprays. Predicted pressure and heat release rate results were compared with engine experimental data and good agreement was observed. The present reduced mechanism gave reliable performance for combustion predictions of RCCI engine operation to help further the fundamental understanding of the process occurring in reformed-fuel RCCI combustion and increase the computational efficiency of multi-dimensional computational fluid dynamics simulations. The reaction mechanism development outlined highlights the importance of considering co-oxidation in generation of reduced reaction mechanisms for applications to dual-fuel combustion.

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1. Introduction

Premixed charge compression ignition (PCCI) combustion strategies are an attractive advanced combustion technique to simultaneously achieve emissions reduction and combustion controllability. Particulate matter (PM) emissions can be reduced by

timing auto-ignition to occur after the fuel and air are mixed below the PM formation threshold and the oxides of nitrogen (NO_x) emissions can be reduced by reducing the combustion temperature by running under highly dilute conditions. Employing the strategy of premixed charge compression ignition, for example, with the use of a fully premixed charge prepared before introduction to the cylinder or a more advanced/retarded direct injection timing than for conventional diesel, this emissions reduction can be successfully achieved [1–8]. Although PCCI combustion is a promising technique to simultaneously achieve high efficiency and low NO_x

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and soot levels, difficulties controlling the combustion phasing and duration have limited their widespread use.

To address these issues Inagaki et al. [9] and Kokjohn et al. [10] proposed blending two fuels with different auto-ignition characteristics inside the cylinder. This in-cylinder blending allows combustion phasing control by varying the ratio of the two fuels and combustion duration control by introducing spatial stratification into the fuel reactivity (i.e., auto-ignition) distribution [15]. Consequently, they termed this alternative combustion mode “reactivity controlled compression ignition,” or RCCI combustion. Kokjohn et al. [10] compared RCCI and conventional diesel combustion in a heavy-duty diesel engine and showed a reduction in NO_x by three orders of magnitude and a reduction in soot by a factor of six. An improvement in gross indicated efficiency by 16.4% was demonstrated due to reductions in heat transfer losses and improved control of combustion phasing and duration. In addition to high efficiency and low emissions, another advantage of RCCI combustion is its fuel flexibility. A number of combinations of conventional and alternative fuels have been studied in RCCI engine combustion [11–14,16–23].

Although dual fuel RCCI combustion shows many beneficial features, the requirement to carry two fuels remains a limiting factor for some applications where a shortage of one fuel causes critical problems. As a viable way to address this technical challenge, utilization of the low reactivity fuel doped with a small amount of appropriate cetane improver to replace the high reactivity fuel has been suggested [24,12]. Splitter et al. [24] used ditertiary butyl peroxide (DTBP) as an additive (up to 3.5% by volume) to pump gasoline and demonstrated the feasibility of using a single fuel as both the high and low reactivity fuels. Hanson et al. [12] used 2-ethylhexyl nitrate (2-EHN) as a cetane improving additive and demonstrated low load single fuel RCCI operation on a heavy-duty engine.

As another method to achieve “single fuel” engine operation, use of an on-board fuel reformer to generate the low-reactivity fuel from a high reactivity fuel stream has been suggested [25]. Based on the thermodynamic analysis of thermochemical exhaust heat recuperation performed by Chakravarthy et al. [26], thermochemical recuperation to drive the endothermic fuel reforming reactions can increase the second law efficiency by up to 11%. Further, this approach has the potential to enable RCCI operation with the reformed fuel. The low reactivity syngas generated from the reformer is introduced into the cylinder as a pre-mixture before direct injection of the high reactivity fuel, allowing single fuel RCCI operation with improved fuel flexibility. Combustion phasing and duration of reformed fuel RCCI is controlled by varying the ratio of syngas to the high reactivity fuel and the spray injection strategy.

To develop a reformed fuel RCCI combustion system, computational fluid dynamics based optimization is needed. For optimization purposes, tens of thousands of simulations are required. Accordingly, computational cost prohibits use of detailed reaction mechanisms that consist of several hundred species and several thousand reactions. A common approach used for exploration of new fuel blends is the use of reduced reaction mechanisms created and validated for single fuels. For example, Nieman et al. [23] performed RCCI combustion calculations of blends of methane and diesel fuel using a reaction mechanism developed and validated for *n*-heptane that contained methane reaction pathways. The mechanism reproduced *n*-heptane and methane ignition delay adequately and was deemed acceptable for use. To date, little attention has been paid to predictability of the chemistry interactions between fuels. The work shows that the chemistry interaction of multiple fuels is of great importance when two fuels with substantially different reactivity are used in engine combustion (e.g., in the case of RCCI combustion using diesel fuel and syngas).

In the present study, single fuel RCCI engine combustion with diesel fuel and its reformed gas fuel is studied. In order to model the physical properties of the diesel fuel sprays realistically, a multi-component surrogate model was employed. The oxidation reaction kinetics was modeled using a reduced reaction mechanism for a single representative component for diesel fuel. Employing the GCR combustion model by Ra and Reitz [27], *n*-heptane was selected for the single component chemistry surrogate. The reaction mechanism for *n*-heptane oxidation processes was reduced from a comprehensive mechanism such that the reaction mechanism of syngas oxidation is included as a sub-mechanism. When developing the reduced mechanism, emphasis was put on the interaction of oxidation reaction pathways of multi-component fuels with large reactivity differences. The reduced mechanism was applied to simulate diesel-syngas RCCI engine combustion and predicted results are compared with measured data.

2. Reaction mechanism formulation

2.1. Comprehensive mechanism

A comprehensive detailed kinetic mechanism for *n*-heptane oxidation processes [28] was used as the base mechanism for the present reduced mechanism. The mechanism consists of 540 species and 2526 reactions to fully describe the fundamental chemical processes involved in *n*-heptane oxidation, and has been validated against various experimental data from laboratory devices. In the mechanism, 25 major classes of elementary reactions were identified. Classes 1–9 are associated with the high temperature oxidation and classes 10–25 are linked to the low temperature oxidation.

Fig. 1 shows the flux diagram for fuel (RH) oxidation. A double arrow indicates that the reaction step involves isomerization. The reactions in the dashed line box indicate high temperature reaction pathways, while those in the dash-dotted line box are for low temperature reaction pathways. A double-arrow indicates that the reaction step involves isomerization. In the diagram, RH denotes fuel, R, R', R'', Q and Q' denote alkyl radicals, S, S', and S'' are olefins

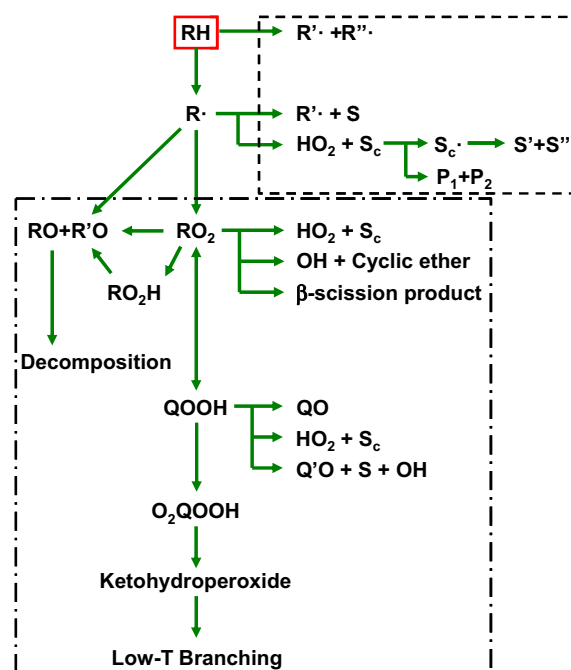


Fig. 1. Schematic representation of *n*-heptane oxidation of Ref. [28].

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