



Optimized chemical mechanism for combustion of gasoline surrogate fuels

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ARTICLE INFO

Article history:

Received 22 August 2014

Received in revised form 12 November 2014

Accepted 13 November 2014

Available online 27 January 2015

Keywords:

PRF/toluene/ethanol

Gasoline surrogate

Optimization

Uncertainty Quantification

ABSTRACT

Since real petroleum fuels are composed of a huge variety of hydrocarbon components, surrogate mixtures of various hydrocarbon fuels are typically employed in computational research and in engine development to represent transportation fuels. In this study, a reduced combustion mechanism of Primary Reference Fuel (PRF) mixtures (*n*-heptane and iso-octane) is integrated into the published kinetic model (Narayanaswamy et al., 2010), allowing for the formulation of multi-component surrogate fuels (e.g. PRF/toluene) and for the prediction of Polycyclic Aromatic Hydrocarbon (PAH) formation in gasoline engines. In order to optimize the model performance, a recently developed optimization technique based on rate rules (Cai and Pitsch, 2014) is extended in this study. The goal is to calibrate automatically the multi-component kinetic mechanism, which also leads to a chemically consistent PRF mechanism and a computational advantage for the calibration process. In addition, this work contributes to the development of general rate rules for various hydrocarbon fuels. An ethanol model is also incorporated into the proposed mechanism. This facilitates the prediction of gasoline/ethanol blend combustion. The resulting mechanism retains a compact size and is successfully validated against experimental measurements.

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1. Introduction

Despite the increasing interest in alternative biofuels, petroleum fuel remains dominant in the transport sector. Nowadays, computational fluid dynamics (CFD) calculations are often applied in engine design to deepen the understanding of the fuel combustion process, for which accurate reaction mechanisms form the backbone [1–3]. While several global properties of practical fuels, e.g. octane number and energy density, can be either experimentally determined or numerically calculated, the detailed combustion kinetics of fuels are highly sensitive to constituents and therefore very complex. Regarding this, surrogate mixtures composed of several hydrocarbon fuels are often used in CFD simulations to represent these real fuels [4]. For gasoline fuel, generally used in spark-ignition and homogeneous charge compression ignition (HCCI) engines, the Primary Reference Fuel mixture of *n*-heptane and iso-octane is often suggested as the surrogate mixture [5,6]. To account for aromatic compounds in petroleum fuel, ternary mixtures of *n*-heptane, iso-octane, and toluene can also be found in numerous published studies to represent gasoline [7–11]. A kinetic mechanism for these surrogate mixtures should

on the one hand enable high-fidelity modeling of individual fuel components and should on the other hand reflect the combustion properties of surrogate mixtures and practical fuels correctly.

A variety of kinetic mechanisms for PRF and ternary mixtures are available in the literature [5,8,12–14]. Curran et al. developed detailed kinetic mechanisms for *n*-heptane [15] and iso-octane [5] oxidation. The combined PRF mechanism has been applied successfully in simulations of homogeneous compression ignition engines [16]. Due to the large number of chemical species and reactions found in the mechanism, several reduced mechanisms were published based on that detailed PRF mechanism [6,17]. A detailed kinetic model for toluene oxidation was derived by Pitz et al. [18], and chemical mechanisms of *n*-heptane/iso-octane/toluene mixtures were studied in various publications [8,19,20]. An interesting additive to surrogate mixtures is ethanol, with which the surrogate fuel can also describe gasoline/ethanol blends in spark ignition engines [21–24]. Cancino et al. [21] and Andrae [25] proposed chemical mechanisms including the combustion chemistry of *n*-heptane, iso-octane, toluene, and ethanol. However, as the chemical reactions of several fuel species are included in the mechanism, both mechanisms consist of more than one thousand species and four thousand reactions. Nevertheless, the detailed reaction chemistry for PAH and nitrogen oxides (NO_x) formation, which is of great interest for engine simulations, is missing in the

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mechanisms. In addition, only ignition delay times were considered as validation targets in these studies. A lumped reaction mechanism was developed by Dirrenberger et al. [23] for *n*-heptane, iso-octane, toluene, and ethanol as well. While the model shows excellent agreement with the measured burning velocities, the validation of ignition delay times is neglected in that study.

In general, a strong variation in constituents can be found for gasoline from various sources. This variation results in different physical and chemical characteristics of gasoline, which affects the formulation of surrogate mixtures. Recently, 1-pentene [12], 2-pentene [13] and di-iso-butylene [25,26] were proposed as additional surrogate components to represent the unsaturated hydrocarbons in gasoline fuels and to minimize deviations of properties between gasoline and the surrogate mixtures. While the choice of the fourth component is highly sensitive to gasoline constituents, a ternary mixture of *n*-heptane, iso-octane, and toluene with an optimized blending ratio is generally able to represent gasoline with different compositions over a wide variety of conditions in CFD calculations, as demonstrated in the literature [27,28]. Therefore, these three surrogate components are considered in this study.

From the standpoint of experimental investigations, a large number of studies for gasoline surrogates can be found in the literature, including measurements of ignition delay times behind reflected shock waves [7,29,30] and in rapid compression machines [9,10], laminar burning velocities [6,31,32], and stable species profiles at different pressures from flow reactors [8] and jet stirred reactors [33].

An additional aspect of the kinetic mechanism development is the continuous refinement of the model accuracy. In the recent years, automatic optimization and uncertainty quantification (UQ) techniques have been successfully established for improving predictive accuracy of chemical schemes [34–37]. In cases of rate parameter optimizations described in the literature, rate parameters of individual reactions are usually systematically optimized to obtain good agreement between experiments and simulations. This can lead to inconsistencies in rate parameters of kinetically similar reactions. Recently, Cai and Pitsch [38] demonstrated a method to calibrate rate rules that determine reaction rates of kinetically similar reactions included in one reaction class instead of rates of single elementary reactions. This leads to a chemically more consistent model calibration. The methodology also reduces the number of active parameters and therefore enables optimization of low temperature auto-ignition, where a large number of reactions appear as important. For the present study, the method is applied to calibrate the PRF kinetic mechanism, in which common rate rules are incorporated for *n*-heptane and iso-octane. Once the general rate rules are automatically calibrated, one would expect that both kinetic models are improved. So far, few studies have focused on the calibration of multi-component mechanisms, and the published studies have been carried out mainly for small species up to C₃H₈ [39,40]. This fact can be attributed to the large number of uncertain but sensitive rate parameters of elementary reactions found in mechanism optimization of large hydrocarbon fuels, which leads to an intractable computational cost. The computational cost will be minimized in this study by using optimization of rate rules rather than individual reactions [38]. This has the advantage that kinetically similar reactions are categorized into classes of reactions with assigned rate rules and that the number of rate rules considered in model development does not increase with the number of fuels in the mechanism. Moreover, the calibration in this study contributes to a refinement of the general rate rules that can be employed to construct hydrocarbon fuel mechanisms.

Nowadays, practical reaction mechanisms for engine design are supposed to model a wide range of hydrocarbon fuels, which are

necessary components of transportation fuel surrogates, with a reasonable mechanism size for CFD simulation. In addition, there is a strong demand for reaction schemes of pollutant formation for emission prognosis and control.

The goal of this study is to propose an accurate and compact chemical mechanism for gasoline surrogate fuel (e.g. PRF/toluene/ethanol). The mechanism is developed in four steps: (a) The PRF and ethanol mechanisms are adopted from the published literature and added as modules on an existing thoroughly-validated model [41] for C₁–C₈ hydrocarbon fuels and substituted aromatic species, e.g. toluene, styrene, *m*-xylene, and 1-methylnaphthalene. This allows for the possibility to propose gasoline surrogate mixtures with various components and to correctly predict PAH formation as well as the further growth to soot particles in engine simulations. (b) For high prediction accuracy, the optimization technique based on rate rules [38] is applied to calibrate the rate rules, which have been employed to construct the multi-component chemical mechanism that is in this study the mechanism of *n*-heptane and iso-octane. The mechanism is optimized against ignition delay times of *n*-heptane, iso-octane, and their mixtures with varying initial compositions over a wide range of conditions. (c) In order to demonstrate the performance of the resulting mechanism, it is extensively tested for laminar flame speeds and jet stirred reactor data for binary PRF mixtures as well as flow reactor data and ignition delay times for ternary mixtures. Subsequently, the ethanol sub-model in the present mechanism is validated against the ignition delay times and the adiabatic burning velocities of ethanol and also the data of ethanol-blended fuels. A large experimental database is used to evaluate the model performance of the oxidation of neat fuels and surrogate blends. (d) Appropriate surrogate model formulations are investigated and discussed in this work.

The presentation of this paper is organized as follows. First, the optimization methodology based on rate rules is introduced. Next, the development of the PRF and ethanol mechanism is described in detail. Then, the proposed mechanism is subjected to the automatic calibration process, leading to an optimized and chemically consistent PRF mechanism. Following this, numerical results using the developed model are presented and compared with experimental data of *n*-heptane/iso-octane/toluene/ethanol mixtures. The paper closes with a short section to assess the surrogate formulation.

2. Methodology

Recently, Cai and Pitsch [38] extended the method by Sheen and Wang [36] for automatic calibration of chemical kinetic models by performing optimization of reaction rate rules. This methodology reduces the number of uncertain parameters by categorizing kinetically similar reactions into reaction classes. It therefore enables the optimization of cases where numerous reactions appear as important, as is the case for low temperature auto-ignition of large aliphatic fuels. A second advantage of this method is that rate rules can be simultaneously optimized for several different fuels and fuel mixtures, which leads to more consistent values for reaction rate coefficients of rate rule. This methodology is described briefly in the following section.

2.1. Reaction classes and rate rules

In the present model development procedure, a well-studied kinetic mechanism including C₀–C₄ chemistry is taken as the base mechanism to describe the oxidation of the small intermediate species generally produced in fuel combustion. Then, the fuel-specific chemistry is derived using prior knowledge of similar

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