Energy Conversion and Management 118 (2016) 44–54

Contents lists available at ScienceDirect

Energy Conversion and Management

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

Numerical investigation of ethanol fuelled HCCI engine using stochastic reactor model. Part 1: Development of a new reduced ethanol oxidation mechanism

Rakesh Kumar Maurya *, Nekkanti Akhil

School of Mechanical, Materials and Energy Engineering, Indian Institute of Technology Ropar, Rupnagar 140001, India

ARTICLE INFO

Article history:
Received 18 December 2015
Received in revised form 20 March 2016
Accepted 25 March 2016

Keywords:
HCCI
Ethanol
SRM
Combustion
Engine

ABSTRACT

Ethanol is considered a potential biofuel for internal combustion engines. In this study, homogeneous charge compression ignition (HCCI) simulations of ethanol engine experiments were performed using stochastic reactor model (SRM). Detailed ethanol oxidation mechanism is developed by including NO_x reaction in existing detailed oxidation mechanism with 57 species and 383 reactions. Detailed ethanol mechanism with NO_x used in this study contains 76 species and 495 reactions. This mechanism was reduced by direct relation graph (DRG) method, which was validated with the experimental results. Existing Lu's 40-species skeletal mechanism with NO formation were also compared with detailed and reduced mechanisms for predicting maximum cylinder pressure, maximum heat release rate and crank angle position of maximum cylinder pressure in HCCI engine. Reduced mechanism developed in this study exhibited the best resemblance with the experimental data. This reduced mechanism was also validated by measured engine cylinder pressure curves and measured ignition delays in constant volume reactors. The results showed that reduced mechanism is capable of predicting HCCI engine performance parameters with sufficient accuracy. Sensitivity analysis was conducted to determine the influential reactions in ethanol oxidation. Results also show that detailed and reduced mechanism was able to predict NO_x emission in good agreement with the corresponding experimental data.

1. Introduction

Hydrocarbon fossil fuels have played an important role in evolution of modern society. Oxidation of fuels generates energy for human needs such as transportation, electricity, etc. Oxidation of fuels also simultaneously generates harmful combustion byproducts. Emission of toxic combustion byproducts into the earth atmosphere leads to air pollution and causes human health issues. Internal combustion engines have large share in consumption of fossil fuels. Fast paced growth in mobility demands further increase in fossil fuel consumptions. To tackle with these challenges, scientific community has two main strategies (i) to replace conventional fuels with alternative and renewable fuels and (ii) shift conventional engine technologies to alternative advanced engine combustion technologies having higher efficiency and ultralow emissions. In second strategy, homogenous charge compression ignition (HCCI) engine mode has been investigated comprehensively by combustion community due to its high thermal efficiency and low emissions [1–4]. HCCI engine combines the best characteristics of conventional spark ignition (SI) and compression ignition (CI) engines. HCCI engine uses homogeneous charge of fuel and air similar to SI engine and the fuel undergoes combustion by auto-ignition similar to CI engine. The major advantages of HCCI engines are higher fuel conversion efficiency in comparison to SI and CI engines of similar displacement volume and extremely low emissions of NO_x and particulate matter (PM) [5]. HCCI engine lacks the direct control of combustion phasing due to autoignition of homogenous charge unlike to conventional SI (spark timing controlled combustion) and CI (mixing controlled combustion) engines. Researchers have used various indirect methods to control the HCCI engine combustion phasing such as intake air preheating [6], dual fuel control [7], variable valve timing [8], exhaust gas recirculation [9], variable compression ratio [10], etc. HCCI engine has limited operating ranges due to higher pressure rise rate during rich mixture engine operation. HCCI combustion mode can be used for commercial application with possibility of switching to conventional combustion mode at higher engine loads. Unburned hydrocarbon (HC) and carbon mono oxide (CO) emissions are typically higher in HCCI mode in comparison to conventional engines

* Corresponding author.
E-mail address: rakesh.maurya@iitrpr.ac.in (R.K. Maurya).

http://dx.doi.org/10.1016/j.enconman.2016.03.076
0196-8904/

because of low combustion temperature but HC and CO can be reduced using aftertreatment technology (oxidation catalytic converter) [11]. Another major challenge in HCCI combustion is cold start of engine, which can be handled by using dual mode (SI-HCCI and CI-HCCI) techniques [12,13].

Due to increasing pollution level in environment and dwindling fossil fuels supplies, biofuels are potential fuels for combustion engines. HCCI combustion mode has flexibility of utilizing any fuel, which can be autoignited in engine cylinder using suitable combustion phasing control strategy. Previous studies have reported that HCCI engine can be operated over wide range of fuels such as ethanol, methanol, butanol, hydrogen, dimethyl ether, biodiesel, etc. [14–19]. Octane number of ethanol is relatively higher in comparison to gasoline, which requires higher combustion temperature for autoignition. Typically alcohols have similar characteristics to that of gasoline with higher oxygen content and can reduce exhaust gas emissions [20,21]. In HCCI engines, ethanol has been used as neat or blends (supplement) fuel [17,19]. Ethanol can operate in HCCI engine on higher speeds than gasoline at lean mixtures [20]. Consequently it would be feasible and better option to use ethanol as fuel in HCCI Engine due to aforementioned advantages.

In order to comprehensively understand HCCI combustion process, models having different level of details are developed using various modelling approaches (single zone models, multiple zone models, computation fluid dynamics (CFD) models) [5]. Multizone models are typically used for investigation of HCCI engines [22,23] due to their capability of predicting the peak pressures and emissions superior than the single-zone models. But multizone models are not perfectly matching the experimental measurements [24] because multizone models fail to consider the fluctuations in zones and chemical source terms are calculated by average temperature and composition in zones. Probability density function (PDF) based approaches such as stochastic reactor model (SRM) attracted increasing attention of researchers in last decade because of their ability to account for in-cylinder mixture composition and temperature stratification in amenable computational timescales [24–26]. In SRM models, the assumption of homogeneity within the cylinder is replaced by one of statistical homogeneity. Physical quantities are described by a PDF, which does not vary within the engine cylinder. Thus, the spatial distribution (due to local inhomogeneities) of the charge is represented in terms of a PDF [24]. SRM has one major difference with CFD models that SRM only accounts for statistical distributions and no spatial information can be obtained. However, due to this simplified approach SRM takes much shorter calculation times. Recent study concluded that SRM has the predictive capability of 3-D CFD codes while simplifying many aspects of CFD processes [27]. Considering the advantages of SRM models and lack of ethanol HCCI model using SRM, present study uses SRM for ethanol HCCI engines.

Detailed kinetic mechanisms or systematically reduced mechanisms are used for prediction of accurate heat release or emitted species for engine parameters for which, only limited or no experimental data available. This increases the capability of engine combustion cycle simulation tool especially for prediction of emissions species [28]. CFD coupled with chemical kinetics is typically used as tool for investigation of the behaviour of intermediate combustion species during ignition and high-temperature combustion in HCCI engines [29]. Studies confirm that HCCI engine emissions can be accurately predicted with sufficient quality of chemical mechanism [30]. Researchers also investigated the distributions of formaldehyde and hydroxyl as well as the coexistence of the species using SRM at the levels beyond detection limit of LIF measurement [31]. One of main objective of this study to investigate the unregulated emission species for ethanol fuelled HCCI engines over wide range of speed and load conditions.

Predictive combustion kinetic model development steps include proper identification of important chemical species and reaction pathways along with collection of relevant rate constant parameters and thermo-chemical data. Current knowledge of ethanol combustion chemistry is contributed for various studies [32–34]. Number of different detailed chemical kinetic mechanism for ethanol exits in published literature that have been tested in different kind of experimental test conditions such as static reactors, shock tubes, flow reactors and premixed flames [34–37]. Recent review paper on modelling HCCI combustion of biofuels presents that all the studies with neat ethanol detailed/reduced mechanism are conducted mostly on single zone and few on multizone and CFD model [14]. Due to absence studies in published literature on reduced ethanol combustion mechanism using SRM, this study is conducted to develop a reduced mechanism using SRM for HCCI combustion engine. Few reduced ethanol mechanisms were mentioned in published review study [14] however these mechanisms were not available in published literature to be used for further analysis. A recent study uses 40 species skeletal ethanol oxidation mechanism with NO formation [38] and mechanism was found on Lu's webpage. Present study also compares the prediction of HCCI combustion parameters with Lu's skeletal ethanol oxidation mechanism [38]. Detailed steps on reduced chemical kinetic development model and details of experimental test conditions for validation of ethanol mechanism is provided in next section.

2. Methodology

2.1. Reduced mechanism development

HCCI combustion is described using set of ethanol oxidation reactions. Detailed chemical mechanism used in this study is a combination of ethanol oxidation mechanism and NOx formation mechanism. The ethanol oxidation mechanism consisting 57 species and 383 reactions from published study [33] is utilized for development of detailed oxidation mechanism for present study. This mechanism does not include the NO_x formation, which is an important regulated species for internal combustion (IC) engines. Nitrous oxide (NO) is major constituent in the exhaust emissions from IC engines. Therefore it is necessary to include the NO_x formation reactions in the ethanol combustion mechanism. A study also investigated the interactions of hydrocarbons on conversion of NO to NO_2 and the effect of NO_x on the oxidation of hydrocarbons [39]. To understand the NO_x formation in ethanol HCCI combustion the Zeldovich mechanism and NO_x reactions from 'GRI MECH 3.0' are included in detailed ethanol oxidation mechanism [40]. Few other reactions are also included from recently published study that provides the important reactions involved in NO_x formation during combustion of hydroxylated fuels [41]. Combining the NO_x reactions to detailed ethanol oxidation mechanism, now the mechanism contains 77 species and 495 reactions. This mechanism is used as detailed ethanol HCCI combustion mechanism in this study.

The size of comprehensive mechanisms sometimes limits their practical utilization because of handling difficulty during computation especially in 3D-CFD. This challenge leads to the development of reduced mechanism, which retains the predictive ability of the complete model with sufficient accuracy over a range of test conditions. Various techniques are used for the reduction of mechanism such as direct relation graph (DRG) [42], path flux analysis [43], principal component analysis [44] and direct relation graph with error propagation (DRGEP) [45]. A study used different methods for developing reduced mechanism also found that DRGEP method fail in some cases [46]. In this study DRG method is used for mechanism reduction. Mechanism reduction is required to