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A skeletal iso-octane reaction mechanism for low temperature plasma ignition with ozone surrogate

Seunghwan Keum*, Cherian A. Idicheria, Paul M. Najt, Tang-Wei Kuo

GM Global Research and Development Center, 30500 Mound Rd, Warren, MI 48090, USA

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Abstract

In this work, we present a skeletal reaction mechanism for modeling ignition of iso-octane with low temperature plasma. The low temperature plasma was modeled by its main product ozone as a surrogate. A key chain branching reaction of oxygen radical attack on iso-octane was identified from reaction pathway analysis. A new skeletal reaction mechanism was developed by incorporating the key reaction along with ozone chemistry to the skeletal iso-octane reaction mechanism from Ra and Reitz [19]. Reaction rate constants of the key reactions and five other related reactions were calibrated to match predictions from the comprehensive reaction mechanism from Curran et al. [*Combust. Flame* 129 (2002) 253–280]. The optimized reaction mechanism shows good agreement with the comprehensive mechanism. It provides sufficient accuracy and computational simplicity to enable practical CFD simulation of low temperature plasma ignition in internal combustion engines.

Keywords: Plasma assisted ignition; Ozone assisted ignition; Reaction mechanism

1. Introduction

With more stringent emission regulations and fuel economy requirements, the paradigm of the gasoline internal combustion engine is shifting toward lean combustion, either with air or exhaust gas recirculation (EGR) dilution. Lean combustion provides better efficiency from higher specific heat capacity ratio and reduced pumping losses. The combustion temperature is lower than stoichiometric combustion, which reduces NOx emissions significantly. However, the level of improvement decreases at higher dilution level because of reduced combustion stability. As the efficiency gain is limited by reduced engine stability at the dilution tolerance, significant efforts have been made to extend the dilution limit using novel ignition systems, such as dual coil igniter [1], microwave ignition [2] and low temperature plasma [3]. The low temperature plasma uses a non-thermal plasma that does not transition to high temperature arc and glow phase. Kadono et al. [3] investigated the ignition and combustion using a low temperature corona discharge with different polarities and reported volumetric ignition and faster combustion than conventional spark, which are beneficial for combustion stability. Shiraishi et al. [4,5] investigated low tempera-

* Corresponding author.
E-mail addresses: seunghwan.keum@gm.com, sgtkeum@gmail.com (S. Keum).

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ture plasma ignition in lean homogeneous charge compression ignition (HCCI) engine and reported superior ignition characteristics than conventional spark discharge. Suess et al. [6] performed experiments with corona ignition device in an HCCI engine and reported superior combustion stability with corona ignition than conventional spark, and extension of dilution limit with the corona ignition. The ignition from a corona ignition device showed volumetric ignition, which generated multiple flame fronts that benefited the combustion stability.

Mechanism of low temperature plasma ignition has been investigated by a number of researchers. Wu et al. [7] measured radical species concentration in the afterglow of a pulsed discharge and reported that low temperature plasma generates radical pool at temperatures as low as 400–800 K. Kosarev et al. [8] reported that the increase in reaction rate was due to chemical effect rather than thermal effect. The electron impact dissociation of oxygen molecules generates highly reactive oxygen radical, which promotes chain branching reactions to increase the reaction rate. The thermal heating from the plasma was reported negligible [8,9]. Breden et al. [10] performed numerical modeling of plasma igniter to investigate the radical yield and their effect on ignition and combustion. However, the computing overhead from the plasma chemistry and related governing equations are yet prohibitive for computational fluid dynamic (CFD) modeling of the plasma igniter in an IC engine.

In the present study, a skeletal reaction mechanism is developed to model the plasma ignition using conventional CFD in IC engine applications. Instead of resolving all plasma chemistry, the non-thermal plasma is modeled by surrogates with oxygen radical and ozone, following Kosarev et al. [8,9]. Conceptually, the surrogate approach is similar to the conventional thermal spark ignition model in IC engine CFD modeling, where the thermal energy is used as a surrogate for the thermal plasma. The oxygen radical yield can be obtained from a separate plasma simulation [10], which can be used as an input to the combustion CFD modeling along with the developed reaction mechanism.

2. Reaction mechanism development: base mechanisms

Curran et al. [11] developed a comprehensive mechanism for iso-octane, which is considered a surrogate for gasoline fuel. The reaction mechanism contains detailed oxygen radical pathways and has been used to understand the effect of oxygen radical in combustion [4]. The detailed reaction mechanism is fairly large with 874 species 3796 reactions, and it is not practical for combustion CFD even with the modern computing resources. Such full mechanisms have been mainly served as a reference for the development and validation of reduced mechanisms that are small enough for CFD simulations.

Recently, efforts have been made to utilize the full mechanisms in CFD by taking advantage of advanced chemistry solvers, for example advanced ordinary differential (ODE) equation solver [12] or tabulated chemistry [13,14]. Contino et al. [15] performed CFD simulation with a large reaction mechanism (1062 species) using advanced tabulated chemistry solver [14] to investigate the effect of ozone seeding on HCCI combustion. However, adaptation of such advanced solver requires significant modification on the CFD code, which is beyond the scope of the current work.

Instead, the current study focused on developing a reaction mechanism that is capable of capturing the effect of oxygen radical, at the same time small enough for CFD applications. There are several methods to reduce a large mechanism to a smaller mechanism [16,17]. However, such mathematical reduction methods have been generally limited to approximately 200 species, which is still too large for engineering combustion CFD applications. Further reduction of a reaction mechanism often involves grouping similar species into a single representative species (isomer lumping) and calibration of reaction rate coefficients [18]. Ra and Reitz [19] proposed a heavily reduced, skeletal primary reference fuel (PRF, a mixture of iso-octane and n-heptane) with 41 species and 130 reactions. The mechanism reduction was first carried out by conventional model reduction methodology, starting from sensitivity analysis, reaction elimination and chemical lumping. Then, the reduced mechanism is further reduced by combining several reactions into one and removing redundant species. Finally, the reaction rate coefficients were calibrated to meet target values. The skeletal mechanism has shown good prediction in gasoline engine modeling with very efficient simulation performance [20]. As such, the skeletal mechanism from Ra and Reitz [19] has been selected as the base mechanism for plasma ignition model development, instead of generating another reduced mechanism from the full mechanism. The skeletal reaction mechanism has sets of reactions for iso-octane, n-heptane, and small hydrocarbon reactions which are common between iso-octane and n-heptane. The present study used only iso-octane and small hydrocarbon reactions with 36 species and 54 reactions.

3. Reaction mechanism development: reaction pathway analysis

A reaction pathway analysis was conducted using the Curran's detailed mechanism [11] to identify key reaction pathway of oxygen radicals. A commercial chemistry solver Chemkin Pro [21] was used for the reaction pathway analysis. Ignition

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