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Research Paper

# Numerical study of combustion characteristics of a natural gas HCCI engine with closed loop exhaust-gas fuel reforming

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## HIGHLIGHTS

- Operating range of natural-gas engines could be extended due to hydrogen addition.
- Reformed exhaust gas recirculation (REGR) was used to produce on-board hydrogen.
- A closed-loop numerical model of a natural-gas HCCI engine with REGR was developed.
- Chemical kinetic analysis of the ignition, combustion and emission were performed.
- Hydrogen addition can advance combustion timing and improve combustion efficiency.

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## ABSTRACT

In order to examine the potential of Natural Gas (NG) engines combining with reformed exhaust gas recirculation (REGR) system, a numerical study was carried out to investigate the combustion characteristics of a NG-HCCI engine with exhaust-gas fuel reforming by using CHEMKIN software. The results indicate that hydrogen added into the cylinder can range from 0.035 up to 0.16. At an equivalence ratio of 0.02 and exhaust gas recirculation (EGR) ratio of 0.2, the indicated mean pressure reaches the maximum and fuel consumption rate reaches the minimum. The hydrogen addition can advance combustion timing and improve the combustion efficiency. Since the exhaust gas offers not only heat but also a certain of CO, $H_2O$, $O_2$, etc., EGR ratio affects the initial conditions during the reforming processes which results in an obvious variation of hydrogen production. It is also found that, with the increase of $H_2$ addition into the cylinder, the H atoms in cylinder is increased, which promotes the generation of $H_2O_2$ and the combustion of engine in advance and more intense. Furthermore, $CO_2$ emission of the engine is affected by both the initial gas conditions in cylinder and the concentrations of CO and H atoms in the inlet gas of engine.



## 1. Introduction

Combining the advantage of the traditional spark ignition and compression ignition, the combustion mode of homogenous charge compression ignition (HCCI) has a very attractive prospect [1]. Meanwhile, as an engine alternative fuel, natural gas (NG) is attracting considerable attention in scientific and industrial community. However, with respect to high auto-ignition temperature characteristics of NG, high compression ratios and intake charge heating are required to achieve the operating conditions in NG engines, which can easily lead to the cylinder knocking and increasing $NO_x$ emissions. Even though the knocking can be inhibited by employing the methods of lean combustion and exhaust gas recirculation (low temperature combustion, LTC), it will cause the engine misfire [2,3]. Because of the unique combustion characteristics of hydrogen such as the wide flammable limit, short minimum quenching distance and fast flame speed, the engine fuelled with the hydrogen-rich mixtures can realize LTC, through which the trade-off can be well solved [4–8]. Therefore, hydrogen addition in a NG-HCCI engine has been extensively studied.

One of the hurdles of the hydrogen-rich combustion technique is how to produce on-line hydrogen. Fortunately, fuel reforming technology and exhaust gas recirculation technology [9,10] (i.e., exhaust-gas fuel reforming technology or reformed exhaust gas recirculation technology: REGR) which can reliably produce on-board hydrogen attracts the attention of researchers. Recently,

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Tsolakis and his co-workers [11–13] experimentally investigated the feasibility of the exhaust-gas fuel reforming technology applied in HCCI engine. The results showed that adding hydrogen into a NG engine through exhaust-gas fuel reforming can not only improve engine combustion but also reduce emissions. Through the technology, for one thing, the exhaust gas heat can be recovered to heat the inlet gas and the hydrogen can be produced by reforming reaction. For another, the unburned hydrocarbon and slipping NG can be controlled as a result of the reforming of hydrocarbons exhausted from the engine and the addition of hydrogen from the reforming. Yap et al. [14,15] considered that the generated hydrogen amount can be kept constant by adding a certain amount of air to adjust reforming gas mixture compositions containing NG, air, $H_2O$ and other reactants. The results indicated that the ignition time could be controlled to a certain range and the required inlet-gas temperature of NG-HCCI engine could be reduced due to the addition of hydrogen.

To the best of our knowledge, the previous NG-HCCI engine with REGR studies focused on the experimental research and the results were mainly explained by the experimental data [16–19]. Actually, the HCCI combustion mode is mainly controlled by chemical kinetics, and thus simulation research by using the CHEMKIN-PRO software can deal with this deficiency, and can further analyse the potential and comprehensively examine the essential reasons of energy conservation and emissions reduction by using REGR from the standpoint of chemical kinetics [20,21].

Therefore, the emphasis of the present study is to simulate the NG-HCCI engine with exhaust-gas fuel reforming by using the CHEMKIN-PRO software with the detailed chemical kinetic mechanism of natural gas. The main parameters including equivalence ratio of inlet-source and exhaust gas ratio (EGR ratio: the ratio of the part exhaust gas circulated into the reformer to the whole engine exhaust gas products) are changed to study their effects on the engine. Finally, these simulation results can be regarded as the theoretical foundation for the following study on the NG engine with exhaust-gas fuel reforming.

## 2. Models and validation

### 2.1. The computational model

As shown in Fig. 1, a closed loop NG-HCCI engine with exhaust-gas fuel reforming was established [22]. The exhaust gas was partly used to provide the heat energy of the reforming process and partly introduced into the reformer of the NG-HCCI engine with exhaust-gas fuel reforming. According to the parameters of the prototype engine from the Refs. [23–25], the engine single-zone model and the honeycomb monolith reactor in CHEMKIN-PRO software were employed to develop the combustion and exhaust-gas fuel reforming computational models of the engine, respectively. Then, the main parameters of the engine (type: Medusa single cylinder 4 V) and the honeycomb monolith reactor are shown in Table 1.

The inlet source was the external source of feed gas defined by users expediently. In this model, the fuel of inlet sources is natural gas. It is known that natural gas includes methane and other light hydrocarbons such as ethane, propane, butane and inert gases, and the composition of natural gas varies in a wide range with the different gas reservoir. However, methane is the huge part of natural gas and its proportion often can be up to 90% or more. Moreover, the present study emphasizes on the investigation of the engine with the closed-loop exhaust-gas fuel reforming and the implementation of this closed-loop system in the way of simulation. Hence, the accepted method is used by simplifying the composition of natural gas into single fuel, that is, the natural gas in this model is represented by methane.

Different components were mixed without chemical reactions in the gas mixer module. The honeycomb monolith reactor module was used to define the reactions of inner surface in circular tube, in which the reforming process for generating the mixture with rich hydrogen is of great complexity, involving a series of reactions including Steam Reforming of Methane (SRM), Partial Oxidation of Methane (POM), Complete Oxidation of Methane (COM), Water Gas Shift (WGS) and Carbon Dioxide Reforming of Methane (CDR), as shown in Table 2 [26]. The reforming reaction time is very short (typically less than 0.05 s), and thus reaction process can be regarded as an adiabatic process. Proportion of each side gas extracted from the whole mixture was set in the gas splitter module. The excessive exhaust gas was expelled from product module. PSR (perfectly stirred reactor) was a reactor that simulates steady and transient state reactions of the mixture. Additionally, due to the closure character of engine model in CHEMKIN and the inlet gas coming from the reformer and inlet model, the engine was connected between PSR (C4) and an inlet model. It is important to note that the external EGR was applied in this system and the parameter of EGR ratio was set in C6_Gas splitter module.

The detailed chemical kinetic mechanism of nature gas GRI-Mech 3.0 has been widely applied in published papers [25] on engines with hydrogen addition and the synthesis gas by methane reforming. GRI-Mech 3.0 was developed by University of California including 53 species and 325 reactions and widely used to describe the chemical reactions of C1, C2, C3 and $NO_x$. The application range is very wide at the temperature of 1000–2500 K, the pressure of 0.013–10 atm and the equivalence ratio of 0.1–5. In this mechanism, gas-phase kinetics and surface kinetics respectively display the elementary reactions of combustion in the cylinder and reforming in the honeycomb monolith reactor. Hence, it is

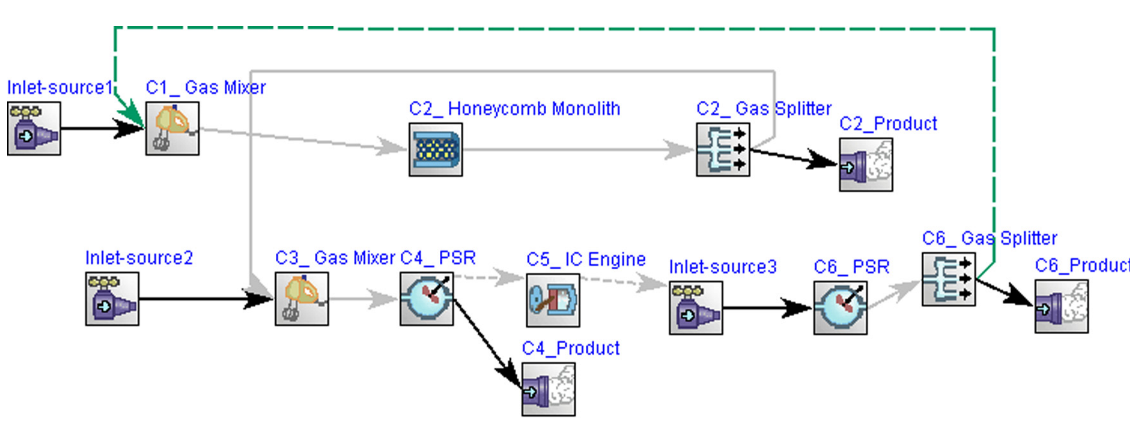


**Fig. 1.** Computational model of the NG-HCCI engine with exhaust-gas fuel reforming.