

Chemical Reaction Processes of Fuel Reformation by Diesel Engine Piston Compression of Rich Homogeneous Air-Fuel Mixture

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ABSTRACT

To extend the operational range of premixed diesel combustion, fuel reformation by piston induced compression of rich homogeneous air-fuel mixtures was conducted in this study. Reformed gas compositions and chemical processes were first simulated with the chemistry dynamics simulation, CHEMKIN Pro, by changing the intake oxygen content, intake air temperature, and compression ratio. A single cylinder diesel engine was utilized to verify the simulation results. With the simulation and experiments, the characteristics of the reformed gas with respect to the reformer cylinder operating condition were obtained. Further, the thermal decomposition and partial oxidation reaction mechanisms of the fuel in extremely low oxygen concentrations were obtained with the characteristics of the gas production at the various reaction temperatures.

The main reformed products were hydrogen (H_2), carbon monoxide (CO), carbon dioxide (CO_2), methane (CH_4), and ethylene (C_2H_4) and the results indicated that the reforming depends on the maximum temperature in the cylinder, however, the amount of reformed gas is lower than the values predicted by the CHEMKIN simulation.

CITATION: Asai, G., Watanabe, Y., Ishiguro, S., Shibata, G. et al., "Chemical Reaction Processes of Fuel Reformation by Diesel Engine Piston Compression of Rich Homogeneous Air-Fuel Mixture," *SAE Int. J. Engines* 10(5):2017.

INTRODUCTION

Diesel engines have become the most commonly used power source for industrial machinery, and along with the strengthening of exhaust emission regulations, much research has been conducted to minimize pollutant emissions. There is strong interest in the development of cleaner combustion modes to utilize thoroughly premixed combustion such as with Premixed Compression Ignition (PCI) and Homogeneous Charge Compression Ignition (HCCI). The HCCI has the potential to achieve extremely low nitrogen oxide (NO_x) and particulate matter (PM) emissions with good fuel consumption. In spite of these advantages, the HCCI combustion still presents issues that must be solved before it would be commercially acceptable. One of the biggest challenges is to establish controllability of the ignition timing throughout the entire range of engine operation [1], [2]. Miyamoto et al. [3] determined aspects of the relationship between fuel ignitability and engine operating conditions such as the compression and EGR ratios. Ohtsubo et al. [4] applied the HCCI combustion to natural gas engines and investigated methods of ignition control by optimization of intake air temperatures and compression ratios. A further HCCI issue is the difficulties with ignition timing control even for similar commercially available research octane number fuels. Here, Shibata et al. [5] have investigated the influence of fuel composition on the heat release characteristics and ignitability.

Another approach to control the ignition timing is using dual fuel (DF) engines, which operate on the lean burn principle of gas engines, although the ignition is controlled by the diesel fuel injection [6]. Presently, DF engines have been introduced mainly for marine propulsion and as auxiliary engines [7]. The DF combustion is a promising technology for a wide range of applications, however, in operation it requires two fuel supply sources, and this is a cause of complexity for the engine system layout and a costly drawback.

With the background as suggested above, research on fuel reforming technology which converts liquid fuels (gasoline and gas oil) into light gases (hydrogen and carbon monoxide) in the engine system, has been actively pursued. Ashida et al. [8] reported on a method of rich gasoline mixture reformation with a catalyst, and Sage et al. [9] discussed the possibility of diesel fuel reformation with partial oxidation, steam reformation, and autothermal reaction by using catalyst reformer. The results showed that the reformed fuel combustion increase the indicated efficiency greater than 4% by the shorter combustion duration and reduced heat losses. And by enabling of the exhaust energy recovery, further improvement of system efficiency can be expected.

Alger et al. [10] introduced the dedicated EGR concept. Here the number one cylinder of four inline cylinders in a gasoline engine is used as a “dedicated cylinder” to operate in the rich condition with an equivalence ratio above 1.0. The purpose of the dedicated cylinder is to provide an increased amount of EGR gas to the other cylinders, with hydrogen and carbon monoxide obtained as by-products. These concepts suggest the possibility of converting liquid fuels into reformed fuels with low ignitability utilizing a rich mixture for the actual combustion.

This study proposes diesel fuel reformation by piston compression to be implemented in the engine to generate reformed fuel which can be utilized for lean homogeneous combustion. For the diesel fuel reformation by using catalyst, the reaction temperature above 1000 K is required to achieve high reformation efficiency [9]. Since the In-Cylinder reformation can produce the high temperature reaction field by piston compression, the higher reformation efficiency can be obtained without additional heating devices.

ENGINE SYSTEM CONCEPT

Figure 1 shows an outline of the components of the engine system used here. Specific cylinders were assigned as reformer cylinder for the reformed fuel production and power cylinders for the combustion of the reformed mixture. A rich mixture with an equivalence ratio above 2.0 is pyrolyzed and partially oxidized at high pressure and high temperature conditions created by the piston compression in the reformer cylinder. As the reformed gas consists of hydrogen (H_2), carbon monoxide (CO), methane (CH_4), with carbon dioxide (CO_2), and water (H_2O), the octane number of the gas is higher than that of conventional diesel fuels. The reformed gas is diluted with air to form a lean homogeneous mixture and introduced into the power cylinders. The injector equipped on the power cylinders supplies a small amount of diesel fuel at the end of the compression stroke to provide an ignition trigger. In this manner lean homogenous combustion can be achieved over a wide speed and load range by optimization of the timing of the diesel fuel injection.

To obtain higher conversion efficiency of the fuel, the intake air of the reformer cylinder are heated by exhaust gas out of power cylinders with heat exchanger. The part of the exhaust energy can be recovered to the reformed gas, an improvement of the system efficiency can be expected.

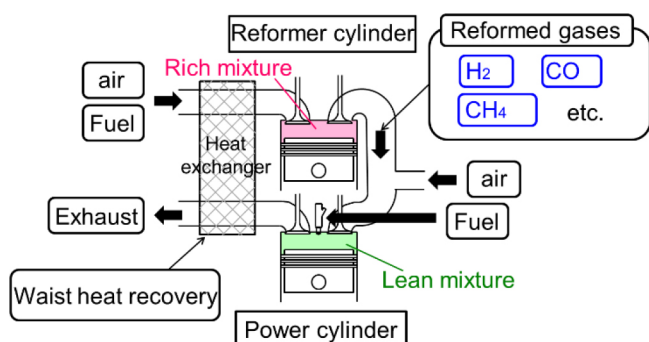


Fig. 1. Engine system concept

DYNAMIC REACTION ANALYSIS

Model Setup

A numerical analysis was carried out to obtain detail of the characteristics of the reformation reaction process and the relationship between engine operation conditions and the composition of the reformed products. The chemistry dynamics simulation software, CHEMKIN Pro, was utilized in this study. The primary input parameter variables for the CHEMKIN simulation are shown in [Table 1](#). The reciprocating cylinder model and the reaction mechanisms of the n-alkane reaction model (2115 species, 8157 reactions) developed by the Lawrence Livermore National Laboratory [11] were used in the simulation. This reaction mechanism contains the detail reaction mechanism of n-alkane up to 16 carbon atoms in the molecule. The dimensions of the cylinder model were set to match the engine used in the experiments. To simplify phenomena, simulations were performed at adiabatic conditions.

The equivalence ratio, and initial temperature are the variable parameters, and the equivalence ratio is adjusted by the oxygen (O_2) concentration in the mixture to maintain the introduction of the same fuel quantities. The equivalence ratios of 2.0 and 5.0 correspond to 10% and 4% O_2 concentrations.

Table 1. Parameter variables for CHEMKIN analysis

Fuel	n-Heptane
Oxidizer	Air
Starting crank angle	-160 °CA ATDC
Calculated crank angle	285 °CA ATDC
Connecting rod ratio	3.51
Displacement	499cm ³
Engine speed	1000 r/min
Initial pressure	1.0 atm
Initial temperature	300-800 K
Compression ratio	18.0
Equivalence ratio	1.0-8.0
Cooling Loss	Adiabatic

Influence of Equivalence Ratio and Initial Temperature

Figure 2 shows the reformed gas concentrations at various equivalence ratios at a 500 K initial temperature. Hydrogen (H_2), carbon monoxide (CO), carbon dioxide (CO_2), and water (H_2O) are dominant in the gas produced at the equivalence ratio of 2.0. With increases in the equivalence ratio, hydrocarbons of smaller molecular weights such as methane (CH_4), ethylene (C_2H_4), and acetylene (C_2H_2) are obtained. At the higher equivalence ratios, the ratios of hydrogen, carbon monoxide and carbon dioxide lowers with increases in the ratio of hydrocarbons. Further, hydrocarbons with 2 or fewer carbon atoms are dominant in the reformed gases at the high equivalence ratios. At the conditions in these simulations, it is considered that large molecule hydrocarbons such as n-heptane are consumed by oxidation or decomposition reactions to form small molecule compounds.

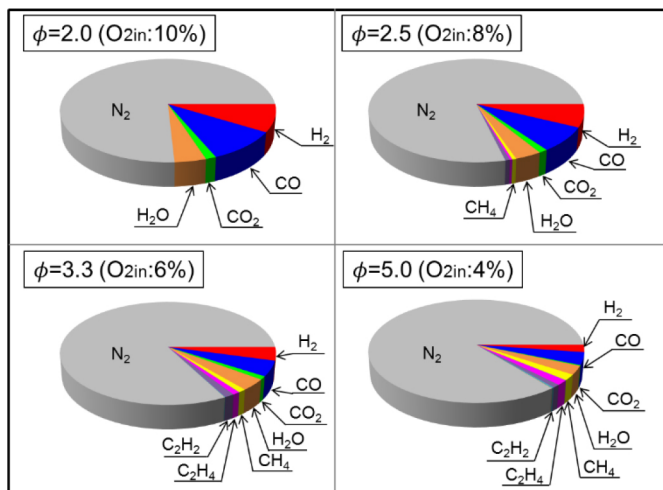


Fig. 2. Estimated mole fractions of reformed gases in $T_{ini}=500\text{ K}$

Figure 3 shows contour plots of the equivalence ratio and initial temperature versus the reformed gas composition, hydrogen, water, carbon monoxide, carbon dioxide, and methane. The areas surrounded by the dashed lines show the area where operation with the single cylinder engine was possible.

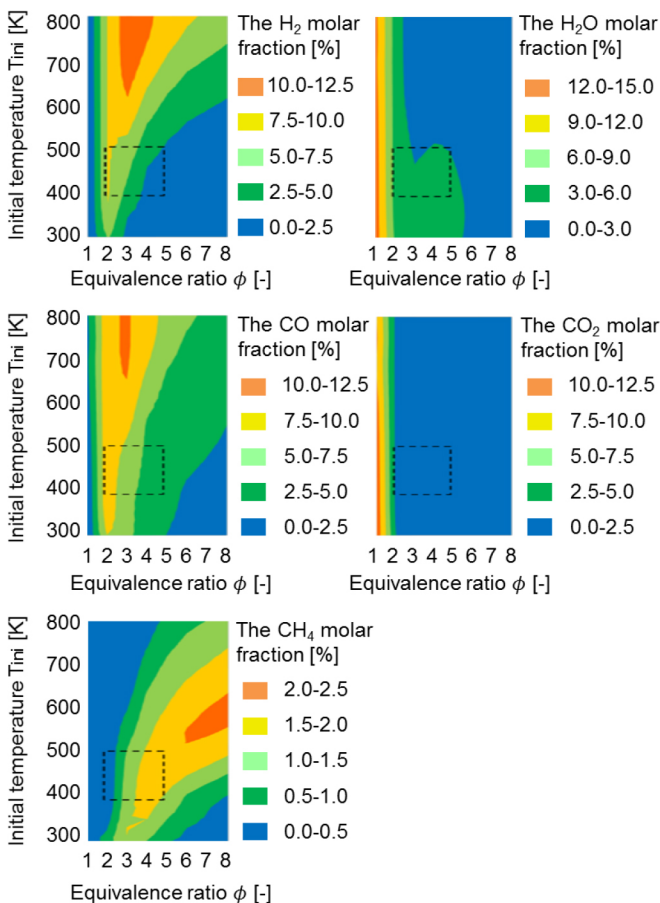


Fig. 3. Characteristics of the produced gas at different equivalence ratios and initial temperatures

The hydrogen reaches the highest value at equivalence ratios of 2-3, and the amounts are proportional to those at the initial temperature. The higher initial temperatures, result in higher concentrations of hydrogen at all equivalence ratios above 2.0. The water shows a largely constant value in the range of equivalence ratios of 2 to 5 and an initial temperature range of 300 K to 500 K. Since the hydrogen is immediately consumed by the water production when there is a sufficient oxygen available, the relationship between hydrogen and water at equivalence ratios below 2.0 shows an inverse correlation. The carbon monoxide shows characteristics similar to hydrogen. It reaches a maximum value in the range of equivalence ratios of 2-4 and higher concentrations are estimated at higher initial temperatures. The oxidation of carbon monoxide is suppressed at lower oxygen concentrations, and carbon dioxide is mainly produced at equivalence ratios below 2.0.

Methane shows different characteristics than hydrogen and carbon monoxide. To obtain higher concentrations of products, higher equivalence ratios are required. The area where methane is produced in Figure 3 is affected by both the equivalence ratio and the initial temperature. Methane molecules are consumed by partial oxidation reactions when there is a sufficient amount of oxygen available, and the methane concentration decreases at lower equivalence ratios. At higher equivalence ratios, the partial oxidation reactions are suppressed by the shortage of oxygen, and concentrations of unreacted hydrocarbons increase. If the temperature is low, the thermal decomposition of hydrocarbons with large molecules is not activate and little methane is produced. At extremely high temperatures, the thermal decomposition of methane molecules becomes active and the methane molar fraction is lowered.

Figure 4 shows the simulated cylinder pressure histories at the different equivalence ratios and initial gas temperatures. In general, the oxidation reaction becomes increasingly active at higher oxygen concentrations, and the reaction rate is higher at lower equivalence ratios. The thermal decomposition of fuel molecules is accelerated by higher ambient temperatures, and an earlier start of the reaction was observed at the higher initial temperatures.

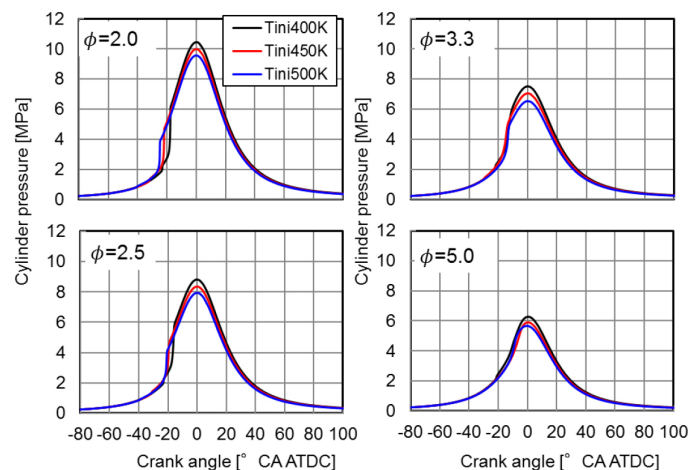


Fig. 4. Simulated cylinder pressure by CHEMKIN

Figure 5 shows the reformed gas molar fractions versus the maximum temperature during the reaction process. The hydrogen (ψ_{H_2}) increases with the maximum cylinder temperature and becomes constant above 2000 K. The carbon monoxide (ψ_{CO}) reaches a local maximum value near 1400 K and increases steadily from 1700 K to 2000 K. The methane (ψ_{CH_4}) and ethylene ($\psi_{C_2H_4}$) reach the maximum values in the vicinity of 1400 K. There are inverse relations between hydrogen, carbon monoxide and methane above 1400 K, and from this it may be assumed that the oxidation reactions that consume hydrocarbons to produce hydrogen and carbon monoxide are increasingly active above 1400 K. Throughout the CHEMKIN simulations, it is suggested that the dominant reactions in the fuel reformation process can be categorized by the maximum cylinder temperature.

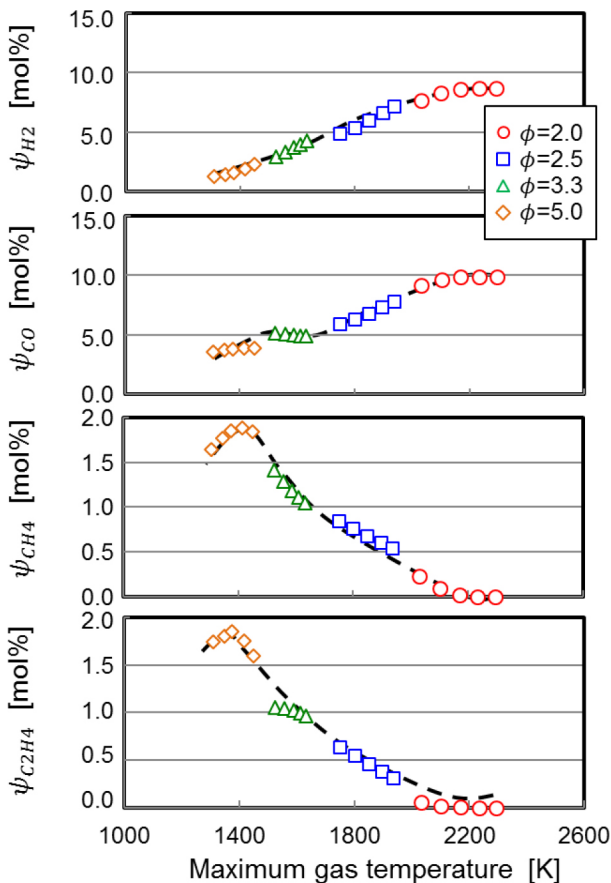


Fig. 5. Reformation characteristics at the maximum gas temperatures

Influence of the Compression Ratio

To investigate the maximum cylinder temperature effects, the compression ratio was chosen as the parameter, and figure 6 shows the simulated maximum cylinder temperatures at the compression ratios 16.1, 18.0, and 20.1 for different equivalence ratios and initial temperatures. The higher maximum gas temperature is obtained at higher compression ratios, lower equivalence ratios and higher initial temperatures. Further, the effects of the compression ratio and the initial temperature on the maximum cylinder temperature are more pronounced at lower equivalent ratios.

The production of hydrogen (a), carbon monoxide (b), and methane (c) at different compression ratios are plotted in Figure 7. Overall the gas production is not strongly influenced by the compression ratio, however the amounts of the reformed gases are influenced markedly.

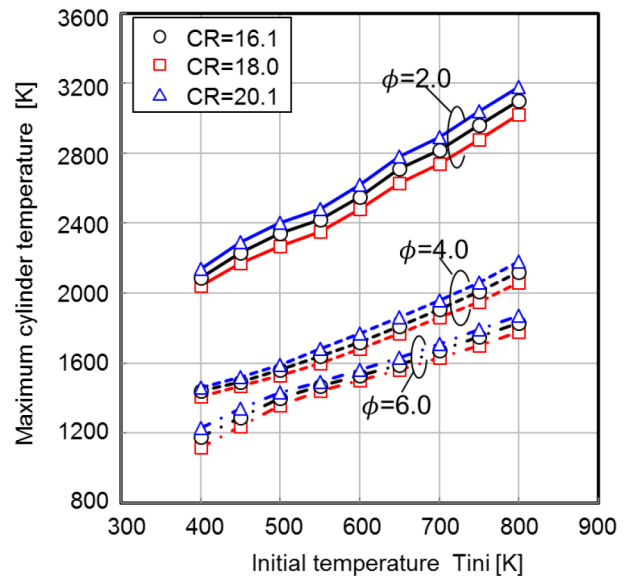


Fig. 6. Plot of simulated maximum cylinder temperatures at various compression ratios, equivalence ratios, and initial temperatures

In Figure 7 (a), the area of higher hydrogen concentrations expands toward lower initial temperatures and higher equivalence ratios. Figure 7 (b) shows similar characteristics, suggesting that higher carbon monoxide concentrations may be expected at higher compression ratios.

In Figure 7 (c), the area of high methane concentrations is shifted to the lower temperature side at high compression ratios. This may be explained by Figure 5 where the methane concentration reaches the maximum value at the maximum cylinder temperature of 1400 K. If the compression ratio is increased, a lower initial temperature would be required to maintain the same maximum cylinder temperature. As discussed with Figure 6, the sensitivity of the compression ratio to the maximum cylinder temperature is stronger at lower equivalence ratios. However, no significant changes in the production of gases were observed in the area of lower equivalence ratios in Figure 7 (a), (b), (c).

The simulated results shown in Figure 5, 6, 7 suggest that for large amounts of hydrogen and carbon monoxide, operating conditions with higher maximum cylinder temperatures are necessary; and to obtain more hydrocarbons such as methane and ethylene, maintaining 1400 K as the maximum cylinder temperature through the optimization of the operating condition is required. In addition, the contribution of the reformed gas composition increase in the order of compression ratio, initial temperature, and equivalence ratio.