In this research, the influence on natural gas combustion of H₂ and CO was investigated by numerical calculations with elementary reactions. The investigation was carried out using the following procedures: 1. To research basic oxidation characteristics of CH₄/H₂/CO mixed fuel, parametric calculations for initial temperature were carried out. 2. For investigation of the effect of H₂ and CO on CH₄ combustion, the calculations with H₂ and CO initial mole fraction variation was carried out. As a result, it was clarified that the oxidation temperature of CO was higher than that of CH₄ and H₂, the increase of H₂ initial fraction has the effect to advance CH₄ ignition timing, and increase of the CO fraction, under the condition that only CO was added, has the opposite effect of H₂ addition.

Key Words: Combustion, Internal Combustion Engine, Compression Ignition, Natural Gas, HCCI

1. Introduction

The Homogeneous Charge Compression Ignition (HCCI) engine, which has attracted attention as the next generation engine, has problems, such as the control of ignition timing, evasion of knocking, and extension of the operating region(1). For the solution to these problems, many researches have been done(2), (3), and the trial to control the operation of the HCCI engine by using mixed fuels is one of them. In other words, this is the method of controlling ignition timing by changing the mixture ratio between easily ignited fuel and non-easily ignited fuel, and expanding the operating region to high load by avoiding knocking(4).

What was considered as the object of analysis by this research was the combustion of the “Reformed Natural Gas Engine System“(5) proposed by H. Kawamura who is one of the authors. This is the system of the high efficiency engine, which uses as a fuel hydrocarbon and carbon monoxide obtained by collecting exhaust energy and reforming natural gas. Natural gas has a potential to reduce exhaust gas pollution. The greatest feature of this system is reforming natural gas to hydrogen and carbon monoxide, collecting heat energy becomes possible, raising thermal efficiency. Natural gas, which is the original fuel, and hydrogen and carbon monoxide, which were generated by reformation, are diluted by EGR gas supplied into the combustion chamber. Such supplied fuel undergoes the adiabatic compression by a piston, resulting in ignition. The combustion realized here is definitely HCCI combustion. In analyzing this combustion, the acquisition of knowledge about control method of HCCI combustion, especially about the method of mixed fuel HCCI combustion, is expected. Actually, the control technique for HCCI engine using natural gas and its reformed gas attracts attention, and experimental research is done(6). However, the effect of the addition of hydrogen or carbon monoxide is not analyzed in detail from the viewpoint of chemical reactions.

In this research, numerical calculations with elementary reactions were carried out for the analysis of HCCI combustion of natural gas, hydrogen and carbon monoxide, which realized in this system. To the fuel-air mixture of Methane (CH₄), which is the main ingredient of natural gas, and air, hydrogen (H₂) and carbon monoxide (CO) were added, and parametric calculations were done by changing the initial temperature and the initial concentration of H₂ and CO in order to investigate the influence of these two reformed gases on CH₄ oxidation from the viewpoint of chemical reactions.
2. Numerical Calculation Methods

2.1 Numerical calculations with elementary reactions

CHEMKIN II\(^{(7)}\) and SENKIN\(^{(8)}\) codes published by Sandia National Laboratory were used to calculate the chemical kinetics of the elementary reactions. CHEMKIN is a FORTRAN software package whose purpose is to facilitate the formation, solution, and interpretation of problems involving elementary chemical kinetics of the gas phase. SENKIN can be carried out under the given volume change. In this research, the GRI-Mech 3.0 scheme (species: 53, reactions: 325)\(^{(9)}\) was selected as the CH\(_4\) elementary reaction scheme. These calculations were carried out based on the following assumptions 1–4 and using the following governing equations.

(1) A premixed mixture is homogeneous. The pressure, temperature and distribution of chemical species are completely uniform (0 dimensional).

(2) Total mass is conserved before and after reactions.

(3) There is no heat transfer (adiabatic change).

(4) The gas in the cylinder is ideal.

Governing equations\(^{(7)}\)

\[
m = \sum_{k=1}^{K} m_k \frac{dm}{dt} = 0 \quad \text{mass equation (1)}
\]

\[
\frac{dY_k}{dt} = v\omega_k \quad k = 1, \cdots, K \quad \text{species equation (2)}
\]

\[
C_v = \sum_{k=1}^{K} Y_k C_{v,k} \quad \text{mean specific heat at constant volume (3)}
\]

\[
\sum_{k=1}^{K} u_k \frac{dY_k}{dt} \quad \text{chemical heat release (4)}
\]

\[
C_v \frac{dT}{dt} + p \frac{dv}{dt} + \sum_{k=1}^{K} u_k \frac{dY_k}{dt} = 0 \quad \text{energy equation (5)}
\]

\[
pv = RT \quad \text{ideal gas equation (6)}
\]

\(t\): time [sec]
\(m\): mass [kg]
\(m_k\): mass of the \(k\)th species [kg]
\(v\): specific volume [m\(^3\)/kg]
\(W_k\): molecular weight of the \(k\)th species [kg/moles]
\(C_{v,k}\): mean specific heat at constant volume [J/(kg·K)]
\(C_{v,a}\): specific heat at constant volume of \(k\)th species [J/(kg·K)]
\(u_k\): Internal energy of \(k\)th species [J/kg]
\(Y_k\): mass fraction of the \(k\)th species
\(p\): pressure [Pa]
\(T\): temperature [K]
\(R\): gas constant [J/mole·K]

2.2 Validities of 0 dimensional numerical calculations and GRI-Mech 3.0 scheme\(^{(9)}\)

In the calculation results in consideration of detailed elementary reactions of the 0 dimensional model, rapid pressure increase and very high heat release compared with the actual HCCI engine are computed. If an equivalent pressure increase and heat release took place in an actual system, the engine will certainly be destroyed.

By CFD calculations, Morimoto and others at Tokyo Gas Co., Ltd. computed the distribution of temperature or concentration at each crank angle in a combustion chamber. Next, they calculated by dividing this distribution by class and giving different temperature or concentration conditions\(^{(10)}\). In these calculations, the combustion chamber was divided into 27 cells, and the movements of a chemical species and heat exchange between each cell are both assumed as negligible. In this case, 0 dimensional calculation was carried out by giving different initial temperature and initial concentration to each cell, but this calculation is actually classified into 1 dimensional calculation because of the existence of the pressure transmission. GRI-Mech 3.0 scheme was chosen as elementary reaction scheme. The figure of the temperature distribution in the combustion chamber computed from CFD calculations is shown in Fig. 1, and the comparison between pressure history obtained from the experiment and that from 0 dimensional calculation, which performed under assumption of homogeneity and non-homogeneity, is shown in Fig. 2. Figure 2 shows that the calculation results assuming non-homogeneity are equivalent to the results of the actual engine. Under the homogeneous condition, the same initial temperature were set to all of the cells, therefore the result of this condition exactly shows the result of 0 dimensional calculation. In actual combustion chamber of the engine, transportation of chemical species, heat transfer and heterogeneity of temperature and concentration exist. However, as well as the calculation done by Morimoto and others, a different initial temperature and...
Fig. 2  Averaged gas pressure histories of 27 cells calculated in homogeneous and non-homogeneous conditions, and the pressure history acquired from experiment(10)

Table 1  Assumed engine specifications

<table>
<thead>
<tr>
<th>Process</th>
<th>Only one compression &amp; expansion</th>
</tr>
</thead>
<tbody>
<tr>
<td>Displacement</td>
<td>1132 cc</td>
</tr>
<tr>
<td>Bore x Stroke</td>
<td>112 x 115 mm</td>
</tr>
<tr>
<td>Length of conrod</td>
<td>250 mm</td>
</tr>
<tr>
<td>Crank radius</td>
<td>57.5 mm</td>
</tr>
<tr>
<td>Intake valve close</td>
<td>ABDC 48°</td>
</tr>
<tr>
<td>Exhaust valve open</td>
<td>BBDC 48°</td>
</tr>
<tr>
<td>Compression ratio</td>
<td>18.0</td>
</tr>
</tbody>
</table>

an initial concentration can be set to each cell by dividing the combustion chamber into two or more cells, heterogeneous be given, 0 dimension calculation be done at each cell, and it bring it close to the result in an actual engine. In that sense, it is considered that the validities of 0 dimensional numerical calculations and GRI-Mech 3.0 scheme are not low.

2.3 Calculation conditions

The engine specifications assumed in this research are shown in Table 1. These specifications are the same as what was used in the analysis performed at Keio University(2).

Chemical reactions of the reformation of CH4 to H2 and CO are shown in the following reactions.

\[
\text{CH}_4 + \text{CO}_2 \rightarrow 2\text{H}_2 + 2\text{CO} - 260 \text{kJ/mol}
\]

\[
\text{CH}_4 + \text{H}_2\text{O} \rightarrow 3\text{H}_2 + \text{CO} - 225 \text{kJ/mol}
\]

These reactions are endothermic reactions and the heat quantity of the reformed fuels is 30% larger compared with the case of using only CH4. The efficiency of the reformation device changes with temperature conditions etc. and, thereby, the quantity of H2 and CO also changes. In this research, calculations were performed under the conditions shown below.

(1) In the Reformed Natural Gas Engine System(5), 10 mol% of the original CH4 is introduced into the engine without reformation and the remaining 90 mol% enter the reformer. On the other hand, all of the exhaust gas flows through the reformer. In the reformer, at first 50 mol% of CH4 is reformed to H2 and CO by the reaction with CO2, and next 65% of the remaining 50 mol% of CH4 is reformed to H2 and CO by the reaction with H2O. When the original amount CH4 is 1 mol, the reforming reactions are expressed as the following equations.

\[
\begin{align*}
\text{CH}_4 + \text{CO}_2 & \rightarrow 0.5\text{CH}_4 + 0.5\text{CO}_2 + \text{H}_2 + \text{CO} \\
0.5\text{CH}_4 + 0.5\text{H}_2\text{O} & \rightarrow 0.175\text{CH}_4 + 0.175\text{H}_2\text{O} + 0.975\text{H}_2 + 0.325\text{CO}
\end{align*}
\]

After the reformation, the fuels (CH4, H2, CO) are introduced into the engine and among the remaining CO2 and H2O, part is exhausted and part is put into the engine as the EGR gas. Under this calculation condition, the calculation was done in reproducing the gas flow mentioned above. The exhaust gas was considered as the complete combustion gas of CH4/air mixture with equivalence ratio of \(\phi = 1.0\), and was assumed to be used for both of the reformation and EGR. The ratio of a mol number of EGR gas and an initial mole number of total gas was defined as EGR ratio \(\gamma_{\text{EGR}}\), and it was set to 50%. The air put into the engine was assumed to have the composition for CH4/air mixture with equivalence ratio of \(\phi = 1.0\). The remaining CO2 and H2O after the reformation were assumed to use in the combustion chamber. The flowchart of these processes is shown in Fig. 3. The initial pressure was set at \(P_0 = 0.1\) MPa. These calculation conditions were selected based on the initial conditions that were realized in the combustion chamber of the Reformed Natural Gas Engine System(5). The initial temperature range was \(T_0 = 300 \text{ K} - 650 \text{ K}\). The purpose of changing the initial temperature was to check the behaviors of chemical species according to compression ignition.

(2) Effect of initial mole fractions of H2 and CO: To investigate the influence that the addition of the reformed gases H2 and CO has on the HCCI combustion of CH4/air

Fig. 3  Flowchart of pre-mixture formation and composition in the calculations for various initial temperatures
mixture, calculations were performed in which the initial mole fraction of H2 and CO was changed from 0.5% to 10% (the equivalence ratio: $\phi_{H2} = 0 - 0.246$, $\phi_{CO} = 0 - 0.246$). The equivalence ratio of the CH4/air mixture was set at $\phi_{CH4} = 0.3$, initial temperature $T_0 = 500$ K, initial pressure $P_0 = 0.1$ MPa and EGR ratio $\gamma_{EGR} = 63\%$. The reason to set the initial temperature to 500 K was that the pre-mixture without H2 and CO was ignited at compression stroke.

3. Results and Discussions

3.1 Effect of initial temperature

Calculations were performed by changing the initial temperature and using the fuel-air mixture composition shown in Fig. 3. The histories of pressure, temperature, and the rate of heat release regarding the change in initial temperature $T_0$ are shown in Fig. 4. Although ignition did not result in ignition in the range of $T_0 = 300$ K – 400 K, pressure and temperature increase and heat release can be checked after TDC at $T_0 = 425$ K. Moreover, the advancement of ignition timing and the increase of the maximum temperature were seen with the increase of initial temperature. The maximum temperature reached 1 500 K at $T_0 = 450$ K, and 1 650 K at $T_0 = 500$ K. Figure 5 shows the histories of the main chemical species at $T_0 = 450$ K. The mole fractions of OH, CH3, HCHO, and H2O2, which are intermediate products, and those of CO2 and H2O, which are final products, increased along with the temperature. The fraction of H2O2 began to decrease at the timing of the increase of the heat release rate, while the fractions of CH3 and HCHO were rapidly reduced at the time when the heat release rate was the highest. Regarding fuel mole fractions, CH4 and H2 began to decrease at the same time CH3 and HCHO did, but the decrease timing of CO was 2 degrees after that of CH4 and H2.

The consumption ratios of CH4, H2, and CO at each initial temperature are shown in Fig. 6. In this figure, the horizontal axis shows the initial temperature values, the vertical axis on the left side shows the ratio of the mole number remained in the exhaust gas to the initial mole number, and that on the right side shows combustion efficiency. Although CH4 and H2 were almost consumed at $T_0 = 430$ K from which combustion efficiency became 85%, CO was not consumed unless $T_0 = 450$ K at which the efficiency became 100%. Figure 7 shows this relationship from a viewpoint of the maximum temperature in a cycle. The horizontal axis shows the maximum temperature values, and what the two vertical axes show is the same as Fig. 6. When the maximum temperature reached 1 300 K, the combustion efficiency exceeded 85%, and CH4 and H2 were almost consumed. However, CO was not oxidized until 1 500 K. This means that when the bulk temperature in the combustion chamber did not reach
Fig. 7 Relationship between consumption ratios of fuels and maximum temperature

1500 K, unburned CO remained as an emission. This is in agreement with the knowledge on HCCI combustion using a single hydrocarbon fuel[3].

3.2 Influence of H2 and CO initial mole fractions to HCCI combustion of CH4/air mixture

3.2.1 Definition of ignition timing, combustion end timing, and combustion duration

In this research, ignition timing, combustion end timing, and combustion duration were defined by the method by below. The definition method is shown in Fig. 8. In the temperature-pressure diagram, the point that the rate of change of temperature to pressure serves as the maximum (the point that the value, which was twice differentiated the temperature from pressure serves as the maximum) was defined as the start of the combustion. The crank angle, pressure, and temperature in this point were made into ignition timing \( \theta_{ign} \), ignition pressure \( P_{ign} \), and ignition temperature \( T_{ign} \). Next, in the history of the rate of heat release, the point that the value was less than 1 J/deg was defined as the combustion end. The crank angle, pressure, and temperature in this point were made into combustion end timing \( \theta_{end} \), combustion end pressure \( P_{end} \), and combustion end temperature \( T_{end} \). Furthermore, the period of \( \theta_{ign} - \theta_{end} \) was defined as combustion duration.

3.2.2 Effect of H2 initial mole fraction

To the CH4/air mixture at \( \phi = 0.3 \), H2 was added in the range of 0.5 – 10%, and calculations were done under the assumption that \( \gamma_{EGR} = 63\% \). The histories of pressure, temperature, and rate of heat release for the H2 initial mole fractions at 0, 0.5, 2, 4, and 8% are shown in Fig. 9. When the H2 initial mole fraction increased to 0.5%, the ignition timing was advanced by 5\(^\circ\) compared to 0%. In the range of 2 – 8%, however, the advancing effect like at 0.5% was not seen. The maximum values of pressure, temperature, and rate of heat release rose with the increase in the H2 initial mole fraction, and especially at the H2 fraction of 8%, heat release was about 8 times the value at 0%. Figure 10 shows the combustion duration at each H2 initial mole fraction. The ignition timing was advanced and the combustion duration was shortened with the increase of the H2 initial mole fraction. When the H2 mole fraction was made to increase to 10%, the duration was about 1/4 that of 0%. The ignition temperatures for various H2 or CO initial mole fractions are shown in Fig. 11. In the H2 mole fraction of 0.5%, the ignition temperature came...
down to about 30 K, and at 10% also decreased to about 70 K. This phenomenon originates in the advancement of ignition timing.

3.2.3 Effect of CO initial mole fraction To the CH4/air mixture at $\phi = 0.3$, CO was added in the range of 0.5 – 10%, and calculations were done under the assumption that $\gamma_{\text{EGR}} = 63\%$. The histories of pressure, temperature, and rate of heat release for the CO initial mole fractions of 0, 0.5, 2, 4, and 8% are shown in Fig. 12. When the CO initial mole fraction increased to 0.5%, the ignition timing and the histories of pressure, temperature, and rate of heat release hardly changed. In the rage of 2 – 8%, however, the ignition timing was retarded, and at the same time, the peak values of pressure, temperature, and rate of heat release increased. In the CO mole fraction of 8%, heat release was about 4 times the value of that at 0%. Figure 13 shows the combustion duration at each CO initial mole fraction. Although the combustion duration was shortened with the increase in the CO initial mole fraction, the ignition timing was gradually retarded, contrary to the increase of the H2 mole fraction. When the CO mole fraction was increased to 10%, the duration was $1/3$ compared with that at 0%. In Fig. 11, the ignition temperature in the CO mole fraction of 10% was 20 K higher compared with that at 0%.

3.2.4 Influence of H2 and CO initial mole fraction to the oxidation reaction of CH4/air mixture In this section, the effect that the change of the initial mole fractions of H2 and CO has on the process of the oxidation reaction of the CH4/air mixture was investigated.

The mole fraction histories of the main chemical species, under the conditions of $\phi = 0.3$, and both of the H2 and CO initial mole fractions being 0%, are shown in Fig. 14. The mole fractions of OH, CH3, HCHO, H2O2, CO2, and H2O increased with the rising of pressure and temperature, while those of CH3, HCHO, and H2O2 decreased at the timing of heat release. Those of H2 and CO continued increasing during the induction period of ignition, like as HCHO and H2O2.

Next, the oxidation reaction when H2 and CO were added to the CH4/air mixture was investigated. The mole fraction histories of the main chemical species, under the conditions of $\phi = 0.3$, the H2 initial mole fraction being 2%, and the CO initial mole fraction being 0%, are shown in Fig. 15. Compared to Fig. 14, the rate of increase of the mole fractions of OH, CH3, HCHO, and H2O2, which were intermediate species, rose during the induction period of ignition. On the other hand, most mole fraction changes of CO2, H2O, CH4, and H2 were not seen in this period. Figure 16 shows the mole fraction histories of the main chemical species, under the conditions of $\phi = 0.3$, and...
the H$_2$ initial mole fraction being 0%, and the CO initial mole fraction being 2%. Compared with Fig. 14, the rate of increase of the mole fractions of OH, CH$_3$, HCHO, and H$_2$O$_2$, decreased during the induction period of ignition. It is guessed that the effect exerted on the combustion of the CH$_4$/air mixture of H$_2$ and CO depends largely on the generation speed of the intermediate species.

Then, the effect that the initial mole fractions of H$_2$ and CO have on the reaction rates of each elementary reaction was investigated. Figure 17 shows the reaction rates of each elementary reaction at each temperature. What has a high rate of contribution to the oxidation reaction of CH$_4$ was picked up, and the reaction rates, under the conditions that the H$_2$ initial mole fraction and the CO initial mole fraction were set at [0%, 0%], [2%, 0%], and [0%, 2%], are shown in this figure. The numbers described at the head of the reaction formulas in this figure correspond to the reaction numbers in the GRI-Mech 3.0 scheme. About the temperature range of reaction, the reactions other than No.99 and No.10 occur in the lower side of temperature range, when H$_2$ is added. What can be said about every reaction in this figure is that the higher side of the temperature range of reaction was expanded both when H$_2$ is 2% and when CO is 2%. This is because the maximum temperature of the cycle becomes higher with the increase of inlet heat quantity.

The oxidation reaction of CH$_4$ begins by drawing out a H atom (No.98).

\[ \text{OH} + \text{CH}_4 \rightarrow \text{CH}_3 + \text{H}_2\text{O} \quad \text{(No.98)} \]

By the addition of H$_2$, the temperature range of reactions No.116 and No.85 becomes low and this result shows the addition of H$_2$ promote generation of OH radicals. Then CH$_3$ is generated by the reaction No.98.

\[ 2\text{HO}_2 \rightarrow \text{O}_2 + \text{H}_2\text{O}_2 \quad \text{(No.116)} \]
\[ \text{H}_2\text{O}_2 (+\text{M}) \rightarrow 2\text{OH} (+\text{M}) \quad \text{(No.85)} \]

CH$_3$ is consumed by the reactions of No.10 and No.119. When comparing the maximum values of the reaction rates for No.10 and No.119, in the case of [0%, 0%], that of No.119 is about 70 times larger. In other words, the consumption of CH$_3$ by HO$_2$ is dominant. Under these circumstances, CH$_3$O is decomposed by reaction No.57 and a H atom is generated.

\[ \text{O} + \text{CH}_3 \rightarrow \text{H} + \text{HCHO} \quad \text{(No.10)} \]
\[ \text{HO}_2 + \text{CH}_3 \rightarrow \text{OH} + \text{CH}_3\text{O} \quad \text{(No.119)} \]
\[ \text{CH}_3\text{O} (+\text{M}) \rightarrow \text{H} + \text{HCHO} (+\text{M}) \quad \text{(No.57)} \]
HO\textsubscript{2} is generated by reaction No.35 and a chain reaction leading to No.119 occurs.

\begin{equation}
H + O_2 + H_2O \rightarrow HO_2 + H_2O \quad \text{(No.35)}
\end{equation}

When H\textsubscript{2} is added, a H atom is produced by No.84 and by leading to the generation of HO\textsubscript{2} the decomposition of CH\textsubscript{3} is activated.

\begin{equation}
OH + H_2 \rightarrow H + H_2O \quad \text{(No.84)}
\end{equation}

The reactions No.33 and No.38, which are related to the H atom, both reactions promote the consumption of CH\textsubscript{3}. When comparing the maximum reaction rates of both reactions, that of No.38 is 3 times faster. These results show that the generation reactions of the O atom are promoted in the reaction process for the H atom. However, in the consumption reactions of CH\textsubscript{3}, when comparing the range of reaction temperatures of No.10 and No.119, only the range of No.119 is expanded to lower temperature. Therefore the consumption of CH\textsubscript{3} by No.119 is promoted.

\begin{equation}
H + O_2 \rightarrow HO_2 + M \quad \text{(No.33)}
\end{equation}

\begin{equation}
H + O_2 \rightarrow O + OH \quad \text{(No.38)}
\end{equation}

When CO is added, although the H atom is produced by No.99, because the reaction rate constant of No.99 is lower when compared to those of No.84 and No.98, a higher temperature is necessary.

\begin{equation}
OH + CO \rightarrow H + CO_2 \quad \text{(No.99)}
\end{equation}

3.2.5 Influence when the initial mole fractions of H\textsubscript{2} and CO are changed simultaneously

To the CH\textsubscript{4}/air mixture at φ = 0.3, H\textsubscript{2} and CO were added simultaneously within the range of 0.5 - 10\%. and calculations were done under the assumption that γ\textsubscript{EGR} = 63\%. The histories of pressure, temperature, and rate of heat release
Fig. 18 Histories of pressure, temperature and rate of heat release for various H2 and CO initial mole fractions

Fig. 19 Ignition timing for various H2 and CO initial mole fractions

when H2 and CO initial mole fraction were [0%, 0%], [0.5%, 0.5%], [1%, 0.5%], [0.5%, 1%], and [1%, 1%], are shown in Fig. 18. This figure showed the histories of the range of the crank angle between −20° and 20°. At [0%, 0%], although the ignition timing had become faster as compared with that of [0.5%, 0.5%], it was almost the same as that of [0.5%, 1%]. Moreover, the ignition timing was also the same at [1%, 0.5%] and [1%, 1%]. In this mole fraction range, it is guessed that the H2 initial mole fraction was what was governing the ignition timing. However, the peak value of the rate of heat release was increased 20 J/deg due to the increase the CO initial mole fraction. The ignition timing for initial mole fractions of H2 and CO is shown in Fig. 19. The X-axis, Y-axis, and Z-axis show H2 initial mole fractions, CO initial mole fractions, and ignition timing, respectively. When the H2 initial mole fraction was increased and combined with any CO initial mole fraction, the ignition timing became 8° – 10° faster within the range of 0.5 – 1%. When the CO initial mole fraction was increased, the ignition timing became slower only when it was combined with the H2 mole fraction of 0%. Conversely, when it combined with more than 2% of H2, the ignition timing advanced. The ignition temperature for various initial mole fractions of H2 and CO is shown in Fig. 20. The Z-axis shows ignition temperature. When the H2 initial mole fraction was increased and combined with any CO initial mole fraction, the ignition temperature became 60 K – 70 K lower within the range of 0.5 – 1%. When the CO initial mole fraction was increased, the ignition temperature became high only when it was combined with the H2 mole fraction of 0%. Conversely, when it was combined with more than 1% of H2, the ignition temperature became lower.

4. Conclusions

In this research, numerical calculations with elementary reactions were performed for the analysis of the HCCI combustion of natural gas and hydrogen and carbon monoxide, which are realized in the Reformed Natural Gas Engine System. The natural gas was represented as the CH4, which is the main ingredient. To the mixture of CH4 and air, H2 and CO were added and parametric calculations were done by changing the initial temperature and the initial concentrations of H2 and CO in order to investigate the influence of these two reformed gases on CH4 oxidation. The following knowledge was acquired.

(1) When the timing of the oxidation start of H2 and CO was compared, that of CO was later, and the temperature required for oxidation was higher compared with that of H2. CO remained in both the initial temperature and the maximum temperature at which CH4 and
H\textsubscript{2} were completely consumed, without being consumed. CH\textsubscript{4} and H\textsubscript{2} mostly oxidized if the maximum temperature reached 1300 K, but CO did not oxidize unless it reached 1500 K.

(2) When only H\textsubscript{2} was added to the CH\textsubscript{4}/air mixture, ignition timing advanced and the ignition temperature became lower. Conversely, when only CO was added to the CH\textsubscript{4}/air mixture, ignition timing was retarded and the ignition temperature became higher.

(3) The existence of H\textsubscript{2} raised the mole fraction rate of increase of the intermediate species during the induction period of ignition in the reaction process of the CH\textsubscript{4}/air mixture. CO had the opposite effect.

(4) When H\textsubscript{2} is added to the CH\textsubscript{4}/air mixture, the range of reaction temperature is expanded to both lower and higher temperatures. The extension of the range to lower temperatures occurs due to the promotion of the following at lower temperatures: 1) the oxidation reaction of CH\textsubscript{3} by an OH radical, and 2) the consumption reaction of CH\textsubscript{3} by HO\textsubscript{2} produced during the reaction process of a H atom. The extension of the range to higher temperatures occurs due to the increase of the maximum temperature during the cycle by a greater inlet heat quantity. When CO is added, the range of reaction temperature is expanded to higher temperatures for the same reason.

(5) In the combination of low initial mole fraction H\textsubscript{2} and CO, it was thought that the initial mole fraction of H\textsubscript{2} was governing the ignition timing. The acceleration effect of H\textsubscript{2} was remarkable when its concentration was low.

(6) The effects of retarding the ignition timing and raising the ignition temperature by CO were discovered only when there is no existence of H\textsubscript{2}. When H\textsubscript{2} existed, it became clear that ignition timing advanced gradually and ignition temperature became lower by the addition of CO.

References


(9) GRI-Mech, http://www.me.berkeley.edu/gri_mech/