

IGNITION CONTROL IN THE HCCI COMBUSTION ENGINE SYSTEM FUELLED WITH METHANOL-REFORMED GASES

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Abstract

Homogeneous charge compression ignition (HCCI) combustion enables higher thermal efficiency and lower NO_x emission to be achieved in internal combustion engines compared to conventional combustion systems. A new concept HCCI engine system fueled with dimethyl ether (DME) with a high cetane number and methanol-reformed gas (MRG) with high anti-knock properties has been proposed by the author et al. In the system, both DME and MRG are to be produced from methanol by onboard reformers utilizing the engine exhaust heat. It has been shown that adjusting the fraction of the two fuels effectively controls the duration of the low-temperature oxidation and the onset of the high-temperature oxidation in HCCI. The ignition control expands the operable range of equivalence ratio and engine load. Lean combustion by HCCI operation and a waste heat recovery by the fuel reforming utilizing engine exhaust heat achieve a high overall thermal efficiency. While MRG consists of hydrogen and carbon monoxide, the ignition control effect of MRG is attributed mostly to hydrogen. The current paper reviews the characteristics of the HCCI engine system fuelled with methanol reformed gases.

Keywords: HCCI, Ignition Control, Hydrogen, DME, Methanol, Onboard Reforming, Waste Heat Recovery

1. Introduction

It is expected that the use of homogeneous charge compression ignition (HCCI) combustion in internal combustion engines will result in higher thermal efficiency and lower NO_x emission as compared with conventional combustion systems. However, difficulties in controlling the ignition timing in accordance with engine load are preventing HCCI from practical application. Adjusting a proportion of two fuels with different ignition properties has been reported as an effective technique to control the ignition timing in HCCI engine [1]. However, this technique has not been practically used for vehicles because of an inconvenience of carrying two fuels onboard.

On the other hand, dimethyl ether (DME) has been studied as a clean alternative to the petroleum diesel fuel due to its high cetane number and smokeless combustion [2-4]. Since DME can be easily produced from methanol by dehydration [5], there has been reported an idea to use a small amount of DME that was produced from methanol as an ignition improving agent in a methanol direct-injection diesel engine [2]. Methanol also can be thermally decomposed to methanol-reformed gas (MRG) that consists of hydrogen and carbon monoxide at relatively low temperatures. Since both hydrogen and carbon monoxide have high anti-knock properties [6], MRG has been studied as a fuel for spark-ignition engines [7-8].

For this background, a new concept HCCI engine system fuelled with DME and MRG has been proposed by the author et al [9-11]. Because the ignition properties of DME and MRG are largely different, adjusting a proportion of the two fuels can control the ignition timing in HCCI engine fuelled with them. In addition to the ignition control, the system is to produce DME and MRG by onboard methanol reformers utilising exhaust gas heat of the engine as shown in Figure 1. Because reactions to reform methanol into DME and MRG are endothermic, the produced DME and MRG have higher heating values than liquid methanol. Therefore, the methanol reformation using the engine exhaust gas heat can be a technique for recovering waste energy from the engine. A combination of the high engine efficiency by HCCI lean operation and the waste heat recovery can achieve a quite high overall thermal efficiency in the system. The use of the single liquid fuel, methanol, also eliminates the inconvenience of having to carry two fuels onboard and makes HCCI applicable to vehicles.

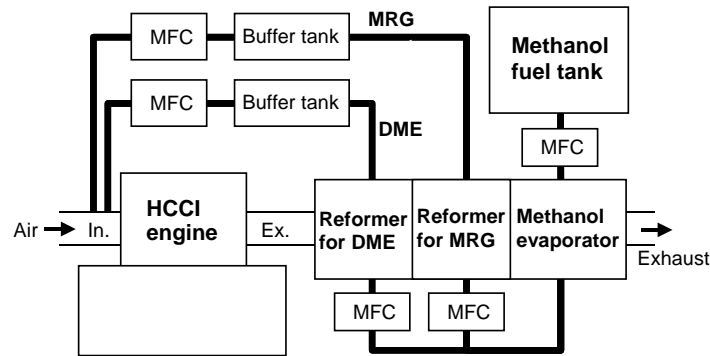
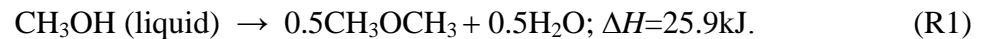


Fig. 1. HCCI engine system fuelled with methanol-reformed gases

2. Methanol reforming reactions

Dimethyl ether (DME; CH_3OCH_3) can be easily produced by catalytic dehydration of methanol (CH_3OH) over gamma-alumina catalysts at quite low temperatures [5].



Because this reaction is endothermic, produced $0.5\text{CH}_3\text{OCH}_3$ has a 4% larger heating value than liquid CH_3OH . Methanol also can be thermally decomposed into 2mol of hydrogen and 1mol of carbon monoxide by the following reaction on an adequate catalyst at relatively low temperatures.



The $2\text{H}_2 + \text{CO}$ has a 20.1% higher heating value than liquid CH_3OH . Therefore, the productions of DME and MRG from methanol using the engine exhaust heat can be a technique for recovering the waste energy.

3. Influence of proportion of DME and MRG

Figure 2 shows characteristics of a HCCI engine that was fuelled with DME and MRG. Influences of a proportion of DME and MRG on indicated mean effective pressure IMEP, indicated thermal efficiency η_i and exhaust emissions against equivalence ratio ϕ are shown in the figure.

The experiments were conducted in a four-stroke cycle single-cylinder engine that has a bore of 85mm and a stroke of 88mm. The compression ratio ε is 9.7. The fuel gases, DME and the MRG model gas stored in high-pressure cylinders were continuously supplied to the intake

manifold of the engine. The MRG model gas consists of 67% hydrogen and 33% carbon monoxide by volume. The MRG fraction in the totally supplied fuel volume was 0, 40, 50 and 60%. The engine speed was set at 1000 rpm. The intake air was at a room temperature without heating.

The figure indicates that larger MRG fraction enables richer combustion and higher IMEP. HCCI operation with DME and MRG demonstrates quite high thermal efficiency over a wider range of operable equivalence ratio and higher IMEP compared to that with neat DME. The concentrations of THC and CO in the exhaust gas tend to decrease as the equivalence ratio ϕ increases. The adjusting the proportion of MRG and DME is very effective to expand the range of operable equivalence ratio in the HCCI engine system.

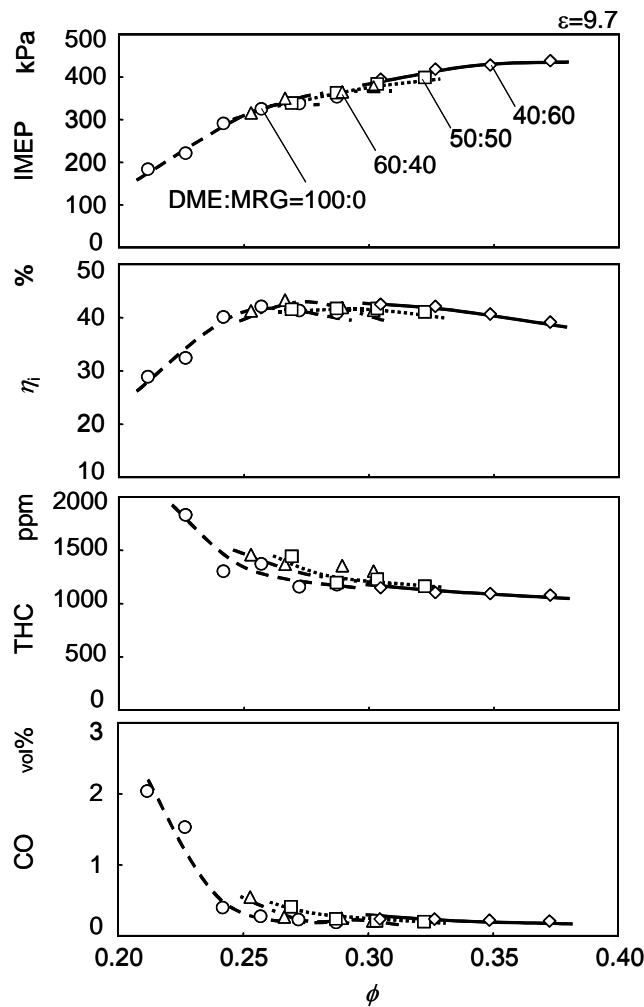


Fig. 2 Indicated mean effective pressure, indicated thermal efficiency and exhaust emissions in a HCCI engine fuelled with DME and MRG

Figure 3 shows indicator diagrams of the HCCI operation with DME and MRG at equivalence ratios that resulted in the highest indicated thermal efficiency for each MRG fraction in the experiments in Figure 2. As shown in Figure 3, the optimum equivalence ratio tends to increase as the MRG fraction increases. Each diagram has a two-stage heat-release pattern with the first-stage by low-temperature oxidation reactions and the second-stage by high-temperature oxidation reactions, which is typical for HCCI combustion of DME. It is clear that the MRG fraction can effectively control the heat-releases in HCCI combustion of DME

and MRG. While the first-stage heat-release is hardly influenced, the second-stage heat-release is significantly influenced by the fraction. An increase in the MRG fraction retards the beginning of the second-stage heat-release that is the main heat-release in HCCI combustion. The retarded main heat-release can avoid a too early combustion phase and a too high pressure-rise in spite of the increased equivalence ratio. These are the reasons for the extension of the operable equivalence ratio range by the MRG addition to HCCI combustion of DME shown in Figure 2.

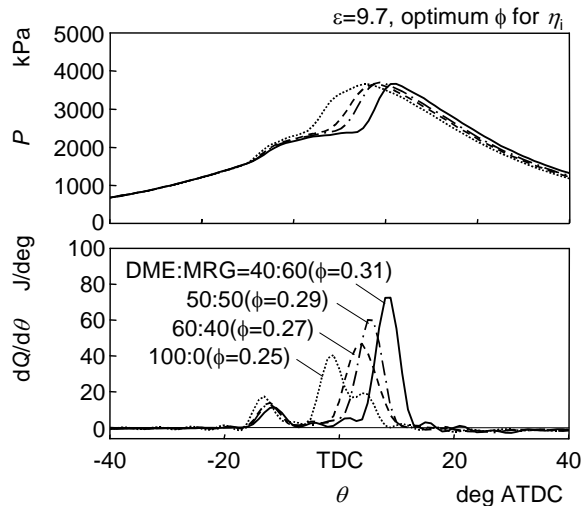


Fig. 3. Indicator diagrams of HCCI engine fuelled with DME and MRG

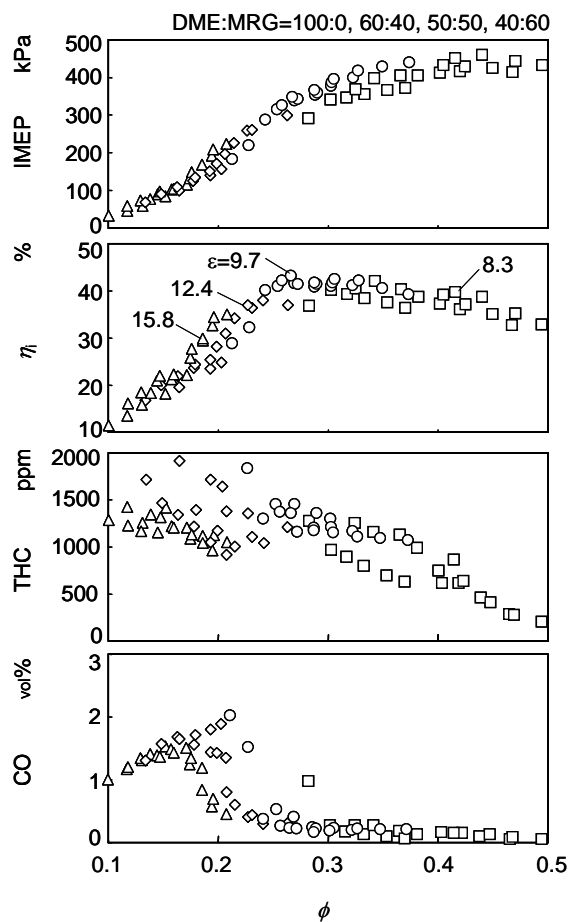


Fig. 4. HCCI combustion of DME and MRG for different compression ratios

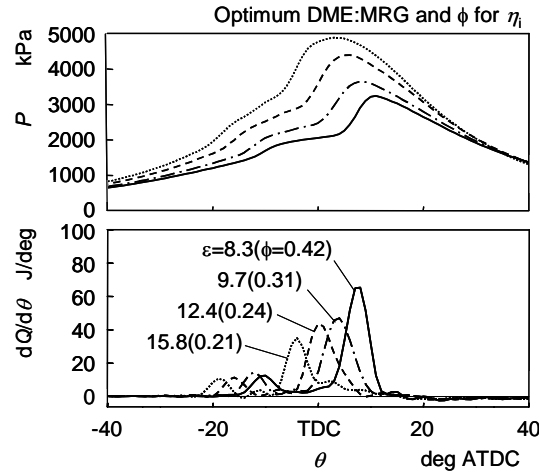


Fig. 5. Indicator diagram of HCCI combustion for different compression ratios

4. Influence of compression ratio

Figure 4 shows characteristics of HCCI combustion of DME and MRG for different compression ratios. The compression ratio ε was varied from 8.3 to 15.8. Combustion limits on the richer mixture side were set by the maximum rate of pressure rise of around 300kPa/°CA. The operable range shifts to richer mixture side as the compression ratio decreases. The compression ratio of 9.7 brings the highest indicated thermal efficiency among the four ratios. Lower compression ratios allow richer combustion with higher IMEP and lower exhaust emissions. The results also suggest a possibility of an ignition control by adjusting the compression ratio in an HCCI combustion engine.

Figure 5 shows indicator diagrams for the each compression ratio. The MRG fraction and equivalence ratio were optimum values for the thermal efficiency. A lower compression ratio retards the beginnings of the both heat-releases by the low- and the high-temperature oxidation. The optimum equivalence ratio increases as the compression ratio decreases, because the retarded heat-release enables richer combustion without causing the too early combustion phase. This is the reason for the higher power output at lower compression ratios in Figure 4.

Figure 6 shows the influence of compression ratio ε on factors influencing the thermal efficiency. The MRG fraction is at 60% by volume and the equivalence ratio is at optimal for the indicated thermal efficiency. The indicated thermal efficiency η_i of an internal combustion engine is expressed by Equation (1) using the theoretical thermal efficiency of the Otto cycle η_{th} , the degree of constant volume η_{glh} , the combustion efficiency η_u and the cooling loss fraction ϕ_w [12-13].

$$\eta_i = \eta_{th} \eta_{glh} \eta_u (1 - \phi_w). \quad (1)$$

The cooling loss fraction ϕ_w and the degree of constant volume η_{glh} can be calculated from the in-cylinder pressure diagram. The measured pressure is influenced by the cooling loss caused by the heat transfer from burning gas to the combustion chamber wall. The cumulative apparent heat-release Q , which is calculated from the measured pressure, is related to the cumulative real heat-release Q_B and the cumulative cooling loss Q_C as follows.

$$Q = Q_B - Q_C. \quad (2)$$

The cooling loss fraction, which is defined as $\phi_w = Q_C/Q_B$, is written as follows.

$$\phi_w = (Q_B - Q)/Q_B. \quad (3)$$

Because the cumulative real heat-release Q_B can be described by a product of the combustion

efficiency η_u and the supplied fuel heat in a cycle Q_{fuel} , the cooling loss fraction ϕ_w can be rewritten with the following equation [13].

$$\phi_w = 1 - Q/(\eta_u Q_{\text{fuel}}). \quad (4)$$

The cumulative apparent heat-release Q can be obtained by integrating the apparent rate of heat-release $dQ/d\theta$ that is calculated with the in-cylinder volume V , the in-cylinder pressure P , the specific heat ratio γ and the crank angle θ as shown in Equation (5).

$$dQ/d\theta = V/(\gamma-1)dP/d\theta + \gamma P/(\gamma-1)dV/d\theta - PV/(\gamma-1)^2 d\gamma/d\theta. \quad (5)$$

Though the term with $d\gamma/d\theta$ in the above equation is often neglected by some researchers, it is known that the term can be quite large during combustion of hydrogen due to its rapid changes in temperature and composition of the in-cylinder gas [14]. Considering the rapid combustion in HCCI engines, the term should be included to the calculation. The degree of constant volume η_{glh} is defined with the apparent rate of heat-release $dQ/d\theta$ by Equation (6) [13-14].

$$\eta_{\text{glh}} = 1/(\eta_{\text{th}} Q) [(1 - ((V_h + V_c)/V)^{1-\gamma}) dQ/d\theta d\theta]. \quad (6)$$

In the equation V_h is the stroke volume and V_c is the clearance volume. The theoretical thermal efficiency η_{th} shown in the figure was calculated with the each compression ratio ε and the specific heat ratio of 1.4 for the Otto cycle. The combustion efficiency η_u in the figure was obtained from the measured oxygen concentration in the exhaust gas.

The indicated thermal efficiency η_i is decreased by an increased cooling loss fraction ϕ_w for compression ratios higher than 9.7 and by a decreased theoretical thermal efficiency η_{th} for compression ratios lower than 9.7. Here, there is no significant change in the degree of constant volume η_{glh} , accordingly the trend of the indicated thermal efficiency η_i is dominated mainly by the theoretical thermal efficiency η_{th} and the cooling loss fraction ϕ_w .

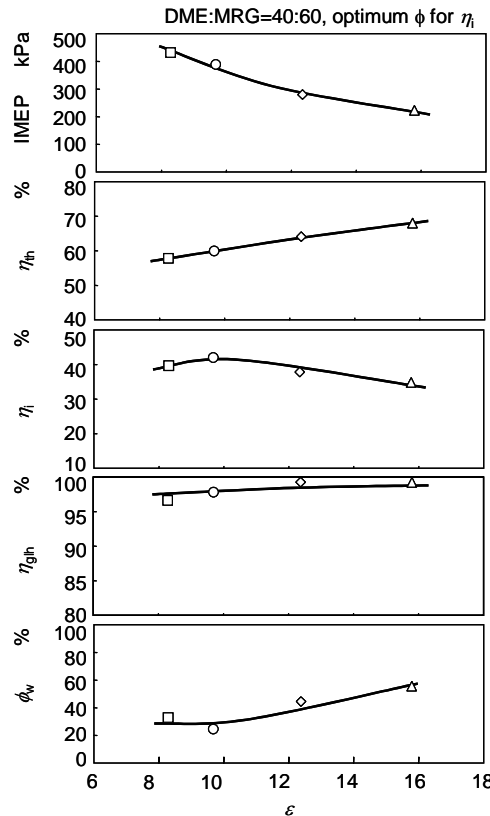


Fig. 6. Influence of compression ratio on thermal efficiency factors

5. Comparison of HCCI and SI

Figure 7 shows a comparison of HCCI and homogeneous charge spark-ignition (SI) combustion at the compression ratio of 9.7. Because of the necessity for a high anti-knock property, SI combustion was fuelled with neat MRG. Ignition was provided by a spark discharge in the central position of the combustion chamber, and set at the optimum timings for the indicated thermal efficiency. The thermal efficiency of the HCCI case is significantly higher than that of the SI case in leaner mixture conditions. Because of the high thermal efficiency, HCCI combustion has a high power output that is comparable to SI combustion in spite of the lean mixture condition. HCCI combustion with excess air ratios lower than 4.0 bring quite low CO exhaust emissions which are similar to the values in the SI combustion case. Although the THC exhaust emission from the HCCI case is higher than that from the SI case, the emission tends to decrease as the excess air ratio decreases. The THC emission could be after-treated by an oxidation catalyst in the practical use of the HCCI combustion engine system.

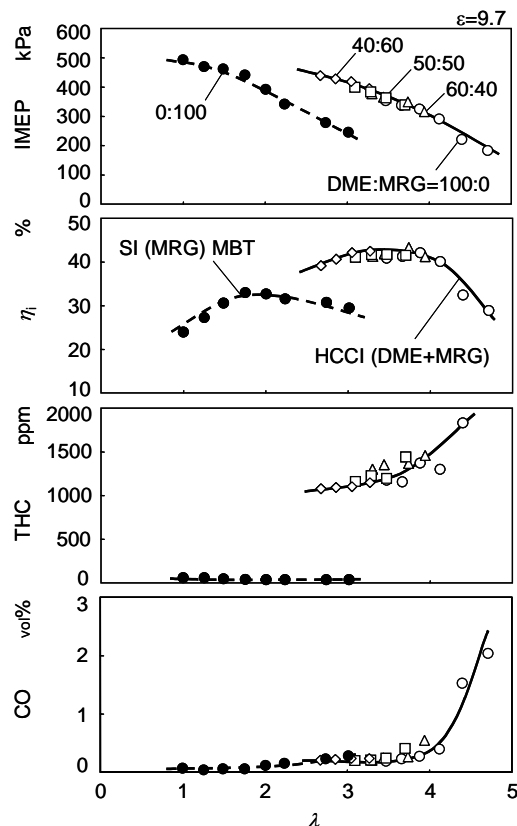


Fig. 7. Comparison of SI combustion and HCCI combustion

6. Overall thermal efficiency including waste heat recovery by fuel reforming

As described in Section 2, DME (CH_3OCH_3) and MRG ($2\text{H}_2+\text{CO}$), which are produced from methanol, have the higher heating values compared to liquid methanol. The utilisation of the engine exhaust gas heat for the endothermic reforming reactions can be a technique to recover the waste heat energy from the engine.

Figure 8 shows the overall thermal efficiency based on the LHV of liquid methanol for the results of HCCI and SI combustion under various operational conditions shown in Figure 7. The index η_r in the figure expresses a degree of the increase in the heating value by the fuel reforming. The value of the index η_r can be calculated for the productions of DME and MRG with following equations respectively.

$$\eta_{r \text{ DME}} = 0.5 \text{LHV}_{\text{CH}_3\text{OCH}_3} / \text{LHV}_{\text{CH}_3\text{OH(l)}}, \quad (7)$$

$$\eta_{r \text{ MRG}} = (2 \text{LHV}_{\text{H}_2} + \text{LHV}_{\text{CO}}) / \text{LHV}_{\text{CH}_3\text{OH(l)}}. \quad (8)$$

The value is 1.04 for the neat DME production and 1.20 for the neat MRG production. The degree of heat increase for the each experimental condition is calculated by Equation (9).

$$\eta_r = \eta_{r \text{ DME}} [\text{DME}] / ([\text{DME}][\text{MRG}]) + \eta_{r \text{ MRG}} [\text{MRG}] / ([\text{DME}][\text{MRG}]). \quad (9)$$

Here, [DME] and [MRG] are volume fractions of DME and MRG to the totally supplied fuel in the experiments. Multiplying the degree of heat increase η_r by the engine efficiency η_i makes the overall thermal efficiency of the system including the waste heat recovery effect by the fuel reforming using the engine exhaust gas.

$$\eta_{\text{overall}} = \eta_r \eta_i. \quad (10)$$

Because the degree of heat increase η_r is higher for the MRG production compared with the DME production, conditions with a larger amount of MRG have advantages in terms of the exhaust heat recovery. The SI combustion, which is fuelled with the neat MRG, has the higher waste heat recovery effect than the HCCI combustion of DME and MRG. However, the overall efficiency $\eta_r \eta_i$ of the HCCI combustion is higher than that of SI combustion, because of the very high engine efficiency by the HCCI operation and the effective exhaust heat recovery. Therefore, it is suggested that the newly proposed HCCI combustion engine system with the waste heat recovery by the onboard fuel reforming is an efficient and clean energy system. The use of the single liquid fuel, methanol, also eliminates the inconvenience of having to carry two fuels onboard while maintaining the effective ignition control by the combination of two fuels with different ignition properties.

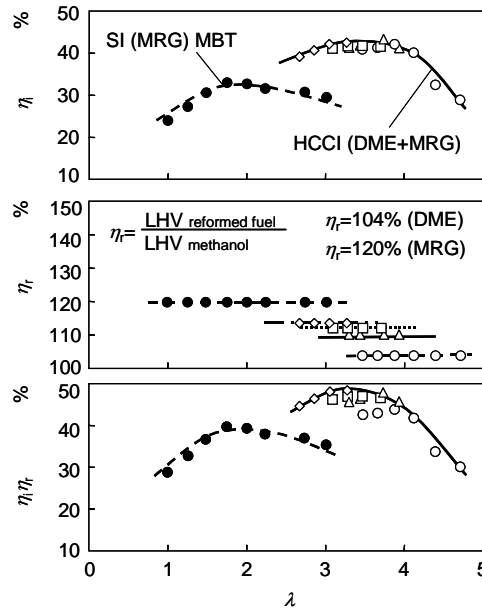


Fig. 8. Overall thermal efficiency including waste heat recovery

7. Ignition control effects by hydrogen and carbon monoxide

While MRG shows the high effect of the ignition control in HCCI combustion of DME, it consists of hydrogen and carbon monoxide. Figures 9 and 10 compare the effects by hydrogen and carbon monoxide. Figure 9 shows a comparison of indicator diagrams with hydrogen and carbon monoxide at a constant DME amount. Figure 10 shows crank angles at onsets of the

heat-releases by low- and high-temperature oxidation reactions (θ_{LTR} , θ_{HTR}), the in-cylinder gas mean temperatures at the timings (T_{LTR} , T_{HTR}) and cumulative apparent heat-releases during low- and high-temperature oxidation reactions (Q_{LTR} , Q_{HTR}). The DME amount was fixed at a value that brings equivalence ratio of 0.27 excluding hydrogen and carbon monoxide.

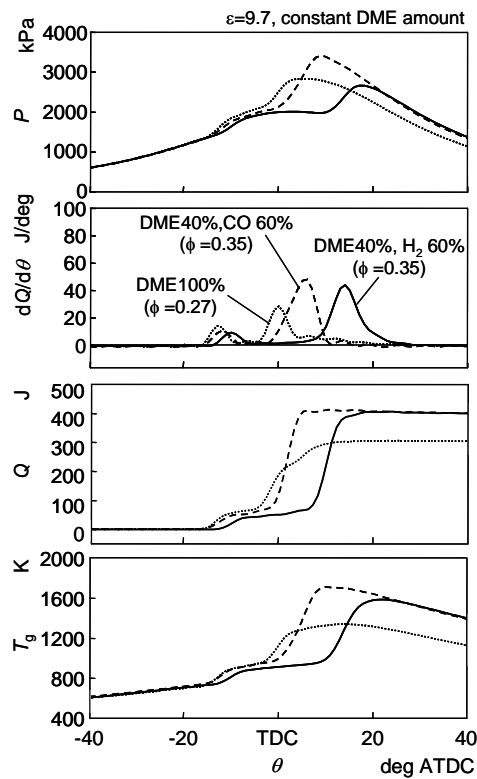


Fig. 9. Comparison of effects by hydrogen and carbon monoxide at constant DME amount

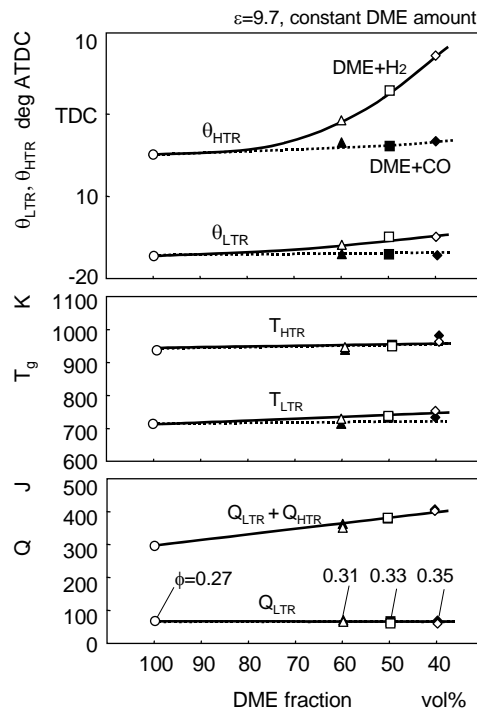


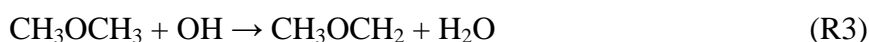
Fig. 10. Comparison of effects by hydrogen and carbon monoxide at constant DME amount

The figures show that the addition of hydrogen or carbon monoxide retards the combustion

phase in spite of the increased equivalence ratio, and it is clear that hydrogen is more effective to control the timing of the second heat-release than carbon monoxide. The ignition control effect by the MRG addition to the HCCI combustion of DME is mostly attributed to the effect of hydrogen. While the hydrogen addition largely retards the timing of the second heat-release, there is no remarkable change in the temperature at the timing. Hydrogen also makes the first heat-release slower and effectively delays the temperature-rise during the low-temperature oxidation of DME. Because of the delayed temperature-rise, the starting-crank-angle of the second heat-release is largely retarded in spite of the no remarkable change in the starting-temperature of the high-temperature oxidation reactions. There is almost no change in the cumulative apparent heat-release during the low-temperature oxidation Q_{LTR} , while the heat release during the high-temperature oxidation Q_{HTR} increases with the equivalence ratio.

8. Reaction mechanism in ignition control

The addition of hydrogen or carbon monoxide to HCCI combustion of DME effectively retards the main heat-release by the high-temperature oxidation reactions. The chemical kinetics mechanism by Curran et al [15-16] is sometimes used to describe the oxidation process of DME, and this mechanism is consistent with previous engine experiments. The first step of the mechanism is the production of CH_3OCH_2 from DME. Though the initiation reaction is the H abstraction from DME by oxygen, the largest part of CH_3OCH_2 is produced by the following H abstraction reaction by OH in the low-temperature oxidation of DME.



The CH_3OCH_2 reacts with O_2 or the third body to produce HCHO, OH and other species. The produced HCHO consumes OH in the following reaction.



The OH is the chain carrier in the low-temperature oxidation. As a result of productions and consumption of the OH, when $d[OH]/dt$ turns negative the chain branching terminates [17]. Hydrogen and carbon monoxide introduced to this low-temperature oxidation process of DME consume OH in the following reactions.



Reaction (R5) has a relatively large rate even in the low-temperature reactions regime. The H produced from the reactions quickly recombines with O_2 to produce HO_2 then HO_2 reacts with H and produces H_2O_2 . However, HO_2 and H_2O_2 are much less reactive than OH during the low-temperature oxidation.



The largely retarded low-temperature oxidation by the addition of hydrogen can be attributed to the consumption of OH by hydrogen. The consumption reduces OH concentration and $d[OH]/dt$. This retards the H abstraction from CH_3OCH_3 by OH that is the main reaction in the first step of the DME oxidation. Subsequently, this delays the heat-release and the temperature-rise during the low-temperature oxidation. While hydrogen does not affect the starting-temperature of the high-temperature oxidation reactions, the onset of the second heat-release delays due to the delayed temperature-rise.

Hydrogen, which largely influences the low-temperature oxidation reactions of DME, is a very effective ignition-controller for HCCI combustion engines fuelled with DME. Adjusting the proportion of DME and hydrogen-containing gases can maintain adequate timings of the

second heat-release without causing the too high rate of pressure-rise in HCCI operations at higher equivalence ratios.

9. Summary

This paper reviewed the characteristics of ignition control, operational range, combustion, thermal efficiency, exhaust emissions, reaction mechanism and possible heat recovery through fuel reforming in the new concept HCCI engine system fuelled methanol reformed gases. The characteristics are summarized as follows:

- The ignition timing is effectively controlled in the HCCI combustion engine system fuelled with DME and MRG by adjusting the proportion of the two fuels. The controlled ignition enables an efficient HCCI operation at a wider range of the equivalence ratio and the engine load as compared with the HCCI combustion of neat DME.
- An increased compression ratio advances the onsets of both first and second heat-releases in HCCI. The advanced ignition timings bring earlier combustion phases and increase the cooling loss by the heat transfer from burning gas to the combustion chamber wall. The optimum compression ratio for thermal efficiency is relatively low as around 10 in the HCCI operation of DME and MRG. By choosing the optimum compression ratio and proportion of DME and MRG, the HCCI operation achieves a higher thermal efficiency and a comparable power output as compared with SI combustion fuelled with MRG.
- An onboard methanol reforming into DME and MRG by utilising the engine exhaust gas heat can be a technique to recover the waste energy and to achieve a quite high overall thermal efficiency in the system. The use of single liquid fuel, methanol, also eliminates the inconvenience of having to carry two fuels onboard while maintaining the ignition control effect by using two fuels with different ignition properties.
- Both hydrogen and carbon monoxide that are contained in MRG have effects to retard the beginning of the second heat-release in HCCI combustion of DME. The effect is far larger in hydrogen addition as compared to carbon monoxide addition. Hydrogen is a very effective ignition controller for HCCI combustion engines fuelled with DME. Adjusting the proportion of DME and hydrogen-containing gases can maintain adequate timings of the second heat-release without causing the too high rate of pressure-rise in HCCI operations at higher equivalence ratios. The ignition control effect of MRG ($2\text{H}_2+\text{CO}$) is mostly attributed to the effect of hydrogen.
- Hydrogen makes the first heat-release slower and effectively delays the temperature-rise during the low-temperature oxidation of DME. Because of the delayed temperature-rise, the starting-crank-angle of the second heat-release is largely retarded in spite of no remarkable change in the starting-temperature of the high-temperature oxidation reactions. The low-temperature oxidation of DME is retarded by a consumption of OH radical by hydrogen. Because the H abstraction from DME by OH radical is the main reaction to produce CH_3OCH_2 in the low-temperature oxidation of DME, the reduced OH concentration effectively retards the early stage of DME oxidation which starts with the H abstraction.

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