Improvement in DME-HCCI Combustion with Ethanol as a Low-Temperature Oxidation Inhibitor

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Abstract

Port injection of ethanol addition as an ignition inhibitor was implemented to control ignition timing and expand the operating range in DME fueled HCCI combustion. The ethanol reduced the rate of low-temperature oxidation and consequently delayed the onset of the high-temperature reaction with ultra-low NOx over a wide operating range. Along with the ethanol addition, changes in intake temperature, overall equivalence ratio, and engine speed were investigated and shown to be effective in HCCI combustion control and to enable an extension of operation range. A chemical reaction analysis was performed to elucidate details of the ignition inhibition on low-temperature oxidation of DME-HCCI combustion.

Introduction

Homogeneous charge compression ignition (HCCI) combustion has attracted much attention due to its potential advantages in achieving ultra lean burning with high thermal efficiency, simultaneous with ultra low emissions of nitrogen oxides (NOx) and particulate matter (PM). However, HCCI combustion meanwhile suffers from a number of weaknesses, principally the difficulty in combustion phasing control, arising from the combustion mechanism of HCCI, where the combustion reaction exclusively depends on the chemistry of the air-fuel mixture. For the ignition control, the use of additives proved to be the most promising and has been proposed by Ricklin et al., who noted that differences in the chemical components or ignitibility could be employed to achieve a wide range of HCCI timing control [1].

With this background, in this paper, ethanol was introduced into a DME fueled HCCI engine from the intake pipe as an inhibitor and the effects of ethanol addition on DME-HCCI combustion were investigated in terms of the onset timings of LTR and HTR (θLTR, θHTR), heat release of LTR ($Q_L$), duration of HTR (HTRD) and operation range. The investigations were at the same time performed under different intake temperatures, and the effect by intake temperature was also illustrated. Finally, the mechanism of the inhibition effect was investigated by the chemical kinetics analysis.

Experiments and calculations

The specifications of the engine used in this study are listed in Table 1, and the experimental apparatus is shown in Fig. 1. Dimethyl ether (DME) was continuously introduced into the intake pipe and ethanol was injected into the intake pipe 0.85 m upstream from the cylinder head to form a highly premixed homogeneous charge. The intake air was electrically heated after the damping chamber, and the temperature of fuel-air mixture at the intake port was constantly controlled. The in-cylinder pressure was measured with a piezoelectric pressure transducer installed in the cylinder head with a time resolution of 0.2ºCA. The output change from the transducer was converted to an amplified voltage. Other operating conditions included an engine speed of 1000 rpm and a coolant temperature of 80ºC.

Definition of combustion parameters

The onsets of LTR and HTR are defined as the points of intersection of the horizontal axis and the tangent of the point where the gradient is the maximum on the respective rising side of the curve of the heat release rate. The end of the LTR is defined as the point where the heat release rate reaches the lowest level after LTR. The end of the HTR is defined as the crank angle corresponding to 20% of the magnitude at the peak of heat release on the falling side of the curve. The duration of HTR (HTRD) is defined as the angle of the interval between the onset and the end of HTR. The heat release during LTR is obtained by integrating the heat release rate during the angle of the interval between the onset and the end of LTR.

Table 1 Engine specifications

<table>
<thead>
<tr>
<th>Engine type</th>
<th>Nissan SC-77</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of cylinders</td>
<td>Single cylinder</td>
</tr>
<tr>
<td>Bore × stroke</td>
<td>85.0 mm × 88.0 mm</td>
</tr>
<tr>
<td>Number of valves</td>
<td>1 inlet valve, 1 exhaust valve</td>
</tr>
<tr>
<td>Displacement</td>
<td>499 cm³</td>
</tr>
<tr>
<td>Compression ratio</td>
<td>10.8</td>
</tr>
</tbody>
</table>
Chemical kinetics

The combustion inhibition mechanism with ethanol in DME-HCCI combustion was analyzed with chemical kinetic modeling, as proposed by Curran et al. [2] and Williams et al. [3]. The CHEMKIN PRO was employed to compute the time evolution of reacting homogeneous gas mixture in a closed system. This system was modeled zero-dimensionally under the assumptions that the gas mixture was completely homogeneous and the reactions occurred in under adiabatic conditions.

Experimental results and discussions

Ignition control with ethanol addition in DME-HCCI combustion

Fig. 2 shows the effects of the ethanol fraction on HCCI combustion of DME under an intake temperature of 20ºC. With the increase in ethanol addition, inhibited LTR and retarded onset of HTR are achieved. This suggests the possibility of a controllable ignition timing that enables combustion to occur in accordance with the operating conditions. The inhibition due to ethanol is further elaborated by observing the onset crank angles of both LTR and HTR, the heat release of LTR ($Q_L$) and the duration of HTR (HTRD) as shown in Fig. 3, where the results with a further two intake temperatures are shown as well.

Inhibition with ethanol in HCCI combustion under various intake temperatures

In Fig. 3, the onset crank angles of both the LTR and HTR are increasingly retarded with the increase in energy fraction of the ethanol addition under a specific intake temperature, and the retardation in HTR is more pronounced than the retardation in LTR. By introducing the ethanol, an extended HTRD can be expected. It is mainly due to the delayed onset timing of the HTR, which makes a part of combustion occur during the expansion stroke. The intake temperature change also changes the mass of the air-fuel mixture under the same equivalence ratio and intake pressure, leading to the decrease in the heat release during LTR. Normally, the increase in temperature accelerates the overall reaction rate following the Arrhenius equation of kinetics. Therefore, the onset crank angles of both the LTR and HTR tend to be earlier, and the HTRD tends to be shorter owing to the increased mean temperature during HTR mainly caused by compression effect before TDC at a higher intake temperature.

Improvement of the rich-side of the HCCI operation range

Fig. 4 shows the expansion of the HCCI operation range on the rich-side with ethanol addition under various intake temperatures. The rich-side combustion limits are determined by the maximum rate of pressure rise of around 1.0 MPaºCA. With the 20ºC intake temperature, the maximum IMEP is successfully extended from
0.352 MPa to 0.521 MPa where the corresponding energy fraction of the ethanol addition reaches to 26.3%. As the intake temperature rises to 40°C and 60°C, the ethanol fraction corresponding to the peak IMEP$_{\text{max}}$ with COV $\leq$ 5% increases from 26.3% to 31.7% and 32.9% separately, however, the peak IMEP$_{\text{max}}$ decreases from 0.521 MPa to 0.480 MPa and 0.430 MPa. Considering the input total energy together with indicated thermal efficiency, this is principally due to the deterioration in indicated thermal efficiency especially in the 40°C case even with the slightly higher energy input at the peak of IMEP$_{\text{max}}$ in the presence of ethanol, as the engine speed increases from 1000 rpm to 1500 rpm and 1900 rpm, the peak IMEP$_{\text{max}}$ is further enhanced from 0.480 MPa to 0.499 MPa and 0.512 MPa under the 40°C intake temperature as shown in Fig. 5.

**Mechanism of the inhibition on low temperature oxidation**

**Ignition control with ethanol addition in DME-HCCI combustion**

Fig. 6 shows the calculated results of the effects of ethanol addition on the HCCI combustion of DME. Here, the overall equivalence ratios of all cases were fixed at 0.26, and the initial temperature for the calculations, $T_{\text{initial}}$ was 345 K. The energy fraction of the ethanol addition to the total input energy was varied from 0% to 20%, the same as the experiments in Fig. 2. The trends of the combustion phase retardation with ethanol addition are similar to that of the experiments. As elaborated by Curran, in the process of the LTR, the reaction sequence governing fuel consumption is an OH reproducing chain mechanism [2]. A summary of the reactions can be expressed as follows [4]:

\[
\text{CH}_3\text{OCH}_3 + \text{OH} = \alpha\text{OH} + \beta\text{CH}_2\text{O + others} \quad (1)
\]
\[
\text{CH}_2\text{O} + \text{OH} = \text{CHO} + \text{H}_2\text{O} \quad (2)
\]

Where $\alpha$ represents the reproduction index of OH, and $\beta$ represents the CH$_2$O formation index. When ethanol is introduced, it consumes OH radicals competitively through the following reactions:

\[
\text{C}_2\text{H}_5\text{OH} + \text{OH} = \text{C}_2\text{H}_4\text{OH} + \text{H}_2\text{O} \quad (3)
\]
\[
\text{C}_2\text{H}_5\text{OH} + \text{OH} = \text{CH}_3\text{CHOH} + \text{H}_2\text{O} \quad (4)
\]
\[
\text{C}_2\text{H}_5\text{OH} + \text{OH} = \text{C}_2\text{H}_5\text{O} + \text{H}_2\text{O} \quad (5)
\]

Fig. 7 shows the rates of production of OH radicals of reactions (3), (4), and (5) under 10% ethanol addition in the energy fraction with other conditions kept the same as those in Fig. 6. As shown here, the three ways of consuming OH radicals work with roughly the same reaction rates. The rate of production of OH radicals by DME is also shown in the figure for comparison. By performing a reaction path analysis to investigate the further products from ethanol in reactions (3), (4), and (5), the products C$_2$H$_4$O and CH$_3$CHOH are found to continue to react with O$_2$ or third body without reproducing OH radicals, however, the C$_2$H$_5$OH in reaction (3) will reproduce the same amount of OH radicals as reaction (3) consumed by simultaneous...
decomposition. Still, overall, the OH radical numbers are decreased with ethanol addition. The change on the OH radicals by ethanol is shown in Fig. 8.

Fig. 7 Rate of production of OH radicals ($\phi_{all} = 0.26$, $T_{initial} = 345$ K, $\Phi_{EtOH} = 10\%$, 1000 rpm)

Fig. 8 Calculated mol fractions of species during LTR of DME-HCCI combustion with different ethanol fractions ($\phi_{all} = 0.26$, $T_{initial} = 345$ K, 365 K and 385 K). The energy fraction of the ethanol addition to the total input energy was varied from 0% to 20%. With wide variations in the computational conditions, the OH radical mol fraction at the onset of LTR is always around $10^{-7}$, and the temperature changes slightly from 772 K to 781 K. Therefore, the OH radical mol fraction may be a critical factor for the onset of LTR.

Fig. 9 shows the calculated OH radical concentration at the onset of LTR for nine conditions with the combinations of three overall equivalence ratios (0.26, 0.36, and 0.46) and three initial temperatures (345 K, 365 K and 385 K). The energy fraction of the ethanol addition to the total input energy was varied from 0% to 20%. With wide variations in the computational conditions, the OH radical mol fraction at the onset of LTR is always around $10^{-7}$, and the temperature changes slightly from 772 K to 781 K. Therefore, the OH radical mol fraction may be a critical factor for the onset of LTR.

Conclusions

1. Under the same overall equivalence ratio, with increasing the energy fraction of ethanol addition into DME-HCCI combustion, the onset of high temperature reaction is increasingly delayed due to the inhibition both on the onset and heat release of the low temperature reaction.
2. By increasing the energy fraction of the ethanol addition, the maximum IMEP of the HCCI combustion under the intake temperature of 20$^\circ$C, was extended from 0.352 MPa to 0.521 MPa. The increase in intake temperature fails to increase the peak of IMEP$_{max}$ higher than 0.521 MPa even with more energy input. The increase in engine speed enables to further enhance the peak of IMEP$_{max}$.
3. The chemical kinetic analysis shows that the OH consumption with ethanol makes the heat release of LTR slower and delays the temperature rise starting the HTR, giving rise to the delayed onset timing of HTR.
4. The OH radical concentration at the onset of LTR is always around $10^{-7}$, where the corresponding gas temperature varies in a narrow range from 772 K to 781 K.

References


Publication