A Spectroscopic Analysis of a Homogeneous Charge Compression Ignition Engine

Hiroki KASUYA, Yoshifumi YAMAZAKI, Seiji OKAMURA, Akira IIJIMA, Hideo SHOJI

Nihon University Graduate School, Nihon University

Homogeneous Charge Compression Ignition (HCCI) combustion offers the advantages of high efficiency and low emissions of pollutants. However, ignition timing control and expansion of the stable operation region are issues remaining to be addressed in this combustion process. Detailed analyses of ignition and combustion characteristics are needed to resolve these issues. HCCI combustion of a low octane number fuel is characterized by two-stage heat release attributed to a cool flame and a hot flame, respectively. In this study, spectroscopic techniques were used to investigate the effect of exhaust gas recirculation (EGR) on ignition and combustion characteristics using a low octane number fuel, which is apt to give rise to a cool flame. The reaction mechanism of a cool flame produces formaldehyde (HCHO). Measurements were made of spontaneous light emission and absorption at wavelengths corresponding to the light emitted at the time HCHO was produced. The light emission intensity and absorbance measured with the spectroscopic techniques revealed clear differences in the cool flame magnitude depending on changes in the EGR rate. It was found that the cool flame magnitude in the HCCI combustion process varied depending on the EGR rate and thus ignition characteristics differed considerably. An investigation was also made of the respective influence on HCCI combustion of high-temperature internal EGR and low-temperature external EGR. The results indicated that external EGR was more effective for retarding the ignition timing, owing to its larger mass per unit volume than that of internal EGR.

Keywords: Engine Combustion / Spectroscopic Techniques, Homogeneous Charge Compression Ignition
compression ratio of 15:1.

<table>
<thead>
<tr>
<th>2-Stroke Air-cooled Single Cylinder Gasoline Engine</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bore x Stroke</td>
</tr>
<tr>
<td>Displacement</td>
</tr>
<tr>
<td>Type of Scavenging System</td>
</tr>
<tr>
<td>Exhaust Port Closing Timing</td>
</tr>
<tr>
<td>Effective Compression Ratio</td>
</tr>
<tr>
<td>Spectroscopic Measurement Internal EGR and External EGR 15:1</td>
</tr>
</tbody>
</table>

Table 1 Specifications of test engine

Fig.1 Light emission and absorbance measurement positions (Compression ratio, \( \varepsilon = 10:1 \))

2.2 TEST FUEL

Ignition of the mixture in an HCCI engine is strongly influenced by low-temperature oxidation reactions. The test fuel used in these experiments for the purpose of ascertaining changes in the state of combustion was n-heptane (0 RON), which exhibits conspicuous low-temperature reactions and is a standard fuel for measuring octane ratings. All of the experiments were conducted at a constant equivalence ratio \( \phi \) of 0.6 in relation to the fresh air.

2.3 ITEMS MEASURED AND MEASUREMENT POSITIONS

The configuration of the experimental equipment used is outlined in Fig. 2. The typical items measured were the cylinder pressure \( P \) (MPa), scavenging temperature \( T_{sc} \) (K), exhaust gas temperature \( T_{ex} \) (K), light emission intensity \( E_{395.2} \) (V) at an emission wavelength of 395.2 nm corresponding to that of formaldehyde (HCHO), which is characteristically produced in a cool flame, and the transmitted light intensity \( E_{293.1} \) (V) at an absorption wavelength of 293.1 nm corresponding to that of HCHO [9-13].

The cylinder pressure was measured with a crystal pressure transducer (denoted as A in Fig. 2) installed in the top of the cylinder head. The scavenging temperature and exhaust gas temperature were measured using K-type thermocouples installed in the scavenging port (denoted as B) and exhaust port (denoted as C). The light emission intensity was obtained by extracting the flame light in the combustion chamber through a quartz observation window (denoted as D in Fig. 1) provided in the top of the cylinder head. Simultaneously, the transmitted light intensity was obtained by irradiating a parallel light beam from a xenon lamp through a quartz observation window (denoted as E in Fig. 1) on one side of the combustion chamber and extracting the transmitted light from a quartz observation window (denoted as F in Fig. 1) on the opposite side. Both the extracted flame light and transmitted light were introduced into monochromators via optical fiber cables, having a core diameter of 1 mm, for separation of the wavelengths of interest. The light at each wavelength was converted to an electric signal by a photomultiplier, and the respective output voltage was regarded as the intensity. The transmitted light intensity at bottom dead center (BDC) was denoted as \( E_{293.1(BDC)} \) (V) and that at an arbitrary crank angle as \( E_{293.1(\theta)} \) (V). Both intensities were converted to absorbance values using Eq. (1) shown below. The wavelength resolution of each monochromator was 4.0 nm in terms the half-bandwidth \( \lambda \).

\[
A_{293.1} = \frac{E_{293.1(BDC)} - E_{293.1(\theta)}}{E_{293.1(BDC)}}
\]

3. DEFINITIONS OF INTERNAL/EXTERNAL EGR RATES

3.1 METHOD OF CALCULATING EGR VOLUME FRACTION

Because of the way in which a 2-stroke engine is built, there is some combustion gas that cannot be removed from the cylinder. In this study, the combustion gas that could be varied intentionally is referred to as the EGR volume fraction. The throttle was set in the wide open throttle (WOT) position, and the differential pressure of the flowmeter was varied by closing or opening the internal EGR valve or the external EGR valve.
For the gas exchange process in the cylinder, a condition of perfect mixing scavenging was assumed in which the incoming fresh air is immediately and completely mixed to form a uniform gas composition. Letting K denote the corrected delivery ratio, the scavenging efficiency \( \eta_s \) (%) at that time is given by

\[
\eta_s = (1 - e^{-K}) \times 100 \% \quad (2)
\]

However, because there is some combustion gas that cannot be evacuated from the combustion chamber, scavenging efficiency \( \eta_s \) when EGR was applied is expressed as \( \eta_s(EGR) \) and as \( \eta_s(Limi) \) when EGR was not applied. The EGR volume fraction \( \gamma_{EGR} \) (%) was approximated using Eq. (3) below [15-16].

\[
\gamma_{EGR} = \eta_{S(Limi)} - \eta_{S(EGR)} \quad (3)
\]

### 3.2 METHOD OF CALCULATING EGR MASS

In calculating the EGR mass, it was assumed that the internal EGR gas temperature was equal to the exhaust temperature and that the external EGR gas temperature was equal to the scavenging temperature. The EGR gas, both internal and external, was assumed to consist of four components: N2, O2, CO2 and H2O. Their volume fractions (\( y_1, y_2, y_3, y_4 \)), molecular weights (\( M_1, M_2, M_3, M_4 \)), critical pressures (\( P_{c1}, P_{c2}, P_{c3}, P_{c4} \)) and critical temperatures (\( T_{c1}, T_{c2}, T_{c3}, T_{c4} \)) were calculated as the respective pseudo values of a mixed gas using Eq. (4) which is Kay’s method [17].

\[
egin{align*}
M' & = y_1 M_1 + y_2 M_2 + y_3 M_3 + y_4 M_4 \quad \text{(g/mol)} \\
P' & = y_1 P_{c1} + y_2 P_{c2} + y_3 P_{c3} + y_4 P_{c4} \quad \text{(Pa)} \\
T' & = y_1 T_{c1} + y_2 T_{c2} + y_3 T_{c3} + y_4 T_{c4} \quad \text{(K)}
\end{align*}
\]

The pseudo-critical constants thus obtained were treated as being equal to the critical constants of a pure gas. The EGR gas density \( \rho \) was estimated with Eq. (5) below and the mass was calculated.

\[
\rho = \frac{P_{EGR} M'}{z R T_{EGR}} \times 10^{-3} \quad \text{(kg/m}^3) \quad (5)
\]

Where \( P_{EGR} \) (Pa) is exhaust gas pressure, \( T_{EGR} \) (K) is exhaust gas temperature, \( R \) (J/mol·K) is a molecular gas constant and \( z \) is the compressibility factor. From a compressibility factor graph, \( z \) was given a value of 1 based on the values of the reduced critical pressure (\( Pr = P_{EGR}/P_{c} \)) and reduced critical temperature (\( Tr = T_{EGR}/T_{c} \)).

### 4. CHEMICAL KINETIC SIMULATIONS

Chemical kinetic simulations were performed using CHEMIKIN 4.0 IC Engine software under dimensionless, adiabatic conditions and by applying the same volumetric changes as those of the test engine. Pressure and temperature data measured experimentally were used as the initial conditions of the calculations. Initial pressure and initial temperature were estimated below.

1. Initial pressure is 0.1 MPa (atmospheric pressure).
2. The in-cylinder gas temperature at the onset of compression \( T_{cpe} \) (K) was defined as shown below as the initial condition of the calculations when internal and external EGR was applied. Letting \( \eta_S \) denote the scavenging efficiency, \( T_{SC} \) the new air temperature (scavenging temperature) and \( T_{EX} \) the residual gas temperature (exhaust gas temperature), \( T_{cpe} \) can be given by the following equation.

\[
T_{cpe} = \eta_S T_{SC} + (1 - \eta_S) T_{EX} \quad (6)
\]

The internal EGR and external EGR compositions are assumed to contain the components produced by burning the mixture having the equivalence ratio of interest. The reduced mechanism for n-heptane [18] proposed by Curran et al. was used as the elementary reaction scheme.

### 5. EXPERIMENTAL RESULTS AND DISCUSSION

#### 5.1 ABSORBANCE AND LIGHT EMISSION INTENSITY

Figure 3 shows the experimental results simultaneously measured for absorbance, light emission intensity and other parameters when EGR was intentionally not applied, and Fig. 4 shows the calculated results of a chemical kinetic simulation.

From the top in Fig. 3, the vertical axes show the cylinder pressure \( P \) (MPa), heat release rate HRR (J/deg.), absorbance \( A_{393.1} \), rate of change in absorbance \( A'_{393.1} \) (deg.\(^{-1}\)), and light emission intensity \( E_{395.2} \) (V) in relation to the crank angle \( \theta \) (deg.) along the horizontal axis. From the top in Fig. 4, the vertical axes show the cylinder pressure, HRR, mole fraction of HCHO and the rate of HCHO production (mol/deg.) in relation to the crank angle along the horizontal axis.

Looking at the results in Fig. 3, it is seen that absorbance increased in the same crank angle interval (region H) in which heat release attributed to a cool flame is observed in the HRR waveform. The calculated results in Fig. 4 show that the HCHO mole fraction increased in the same crank angle interval (region I) in which heat release ascribed to a cool flame is observed in the HRR waveform. These results revealed that a change in the HCHO concentration can be inferred from the absorbance waveform. A comparison of the rate of change in absorbance in Fig. 3 and the rate of HCHO production in Fig. 4 yielded a similar result. Presumably, this indicates that the rate of change in absorbance is effective in confirming the rate of HCHO production and changes in production reactions.

In Fig. 3, a faint light emission is observed in the light emission intensity waveform in the same interval (region H) in which absorbance and its rate of change were both large. From these results, it is inferred that the light emission at 395.2 nm, corresponding to HCHO, in the cool flame region represents light that was emitted in the production reactions of HCHO.
Fig. 3 Basic waveforms (experimental)

Fig. 4 Basic waveforms (calculated)

Fig. 5 Influence of internal EGR (experimental)

Fig. 6 Influence of internal EGR (calculated)

Fig. 7 Influence of external EGR (experimental)

Fig. 8 Influence of external EGR (calculated)
increased in the presence of a cool flame and decreased under a hot flame. It is seen that the respective values (regions a, b, c and d) in the cool flame interval changed as the EGR rate was increased.

The characteristics used in analyzing the absorbance waveforms, rate of change in absorbance waveforms, mole fraction waveforms and rate of production waveforms are defined below, in Fig. 9 and in Fig. 10.

**ALTR/MLTR (Fig. 9):** the absorbance/the mole fraction at the time the absorbance/the mole fraction waveform increased gradually (point X/Y) concomitant with the occurrence of the cool flame.

**θA-LTR/θM-LTR (Fig. 9):** the crank angle at the time of the ALTR/MLTR.

**A'MAX/ROPMAX (Fig. 10):** the maximum value of the rate of change in absorbance/the rate of HCHO production (point X'/Y') at the time the cool flame occurred.

**θA'-MAX/θROP-MAX (Fig. 10):** the crank angle at the time of the A'MAX/ROPMAX.

A comparison of the experimental and calculated results reveals that both absorbance and the HCHO mole fraction, as well as both the rate of change in absorbance and the rate of HCHO production, decreased owing to the increase in the EGR volume fraction. These results suggest that absorption spectroscopy can be used to estimate the change in the HCHO concentration even when EGR is applied and that the rate of change in absorbance is effective in confirming changes in the rate of HCHO production and in the production reactions.

Figure 11 shows the light emission intensity waveforms that were obtained when different levels of internal EGR were applied and Fig. 12 shows the corresponding results when external EGR was applied. Looking at the faint light emission concomitant with the occurrence of a cool flame (region J), the light emission was no longer observable once the volume fraction of either internal or external EGR reached 15%. The reason for that is presumed to be a reduction of the quantity of...
HCHO produced and its rate of production at the time the cool flame occurred, owing to a decrease in the effect of EGR and the amount of fuel supplied. In other words, in addition to the influence of the temperature and concentration, the faint light emission attendant upon the cool flame can be observed when the HCHO production reactions are active. Additionally, absorption spectroscopy is capable of capturing changes in the concentrations of intermediate products resulting from low-temperature oxidation reactions in the interval when heat release degenerates following the occurrence of the cool flame and before the hot flame develops. Accordingly, the combined use of emission spectroscopy and absorption spectroscopy is effective in gaining a better understanding of low-temperature oxidation reactions.

5.2 VARIATION OF EGR

Figure 13 shows typical examples of the heat release rates calculated for different internal EGR volume fractions, and Fig. 14 shows those calculated for different external EGR volume fractions. Figure 15 shows the change in ignition timing, which is defined as the time of 10% heat release in relation to the maximum heat release rate. The results in Fig. 13 indicate that a cool flame occurs at an increasingly earlier crank angle (arrow K) as the internal EGR volume fraction is increased. The ignition timing, on the other hand, advances to an earlier crank angle at a small internal EGR volume fraction and is then retarded when the volume fraction is increased further. This is indicated by arrow L in Fig. 13 and by the results in Fig. 15. The results in Fig. 14 indicate that a cool flame occurs at nearly the same crank angle (arrow M), regardless of the increase in the external EGR volume fraction, which is different from the tendency seen in Fig. 13. Arrow N in Fig. 14 and the results in Fig. 15 show that the ignition timing is gradually retarded.

For the purpose of examining these results more closely, Fig. 16 shows the relationship between the EGR volume fraction and EGR mass. The high-temperature internal EGR probably quickens the occurrence of a cool flame through its strong effect on raising the in-cylinder gas temperature at the onset of compression. Concomitant with the earlier occurrence of a cool flame under a small internal EGR volume fraction, the ignition timing also advances to an earlier crank angle. However, because of the constant equivalence ratio in relation to the fresh air, the injected heat value is reduced by increasing the EGR volume fraction, which also reduces the quantity of heat released by the cool flame. As a result, the interval from the occurrence of the cool flame to ignition becomes longer. When that tendency becomes stronger than the tendency for the cool flame to occur at an earlier crank angle, the ignition timing presumably begins to be retarded.

Because external EGR is at a lower temperature than internal EGR, it has less effect on raising the in-cylinder gas temperature at the onset of compression. That explains why the time for the occurrence of a cool flame did not change
Additionally, external EGR probably has a stronger inactivation effect than internal EGR because its mass per unit volume is greater than that of the latter. Accordingly, the inactivation effect due to the change in gas composition also worked to retard the ignition timing, in addition to the smaller quantity of heat released by the cool flame as a result of the reduced fuel supply.

The results in Figs. 13 and 14 indicate that the maximum HRR decreased accompanying the increase in the EGR volume fraction. However, because the injected heat value was reduced, the decrease in the maximum HRR does not necessarily signify a suppression of the combustion reaction speed (maximum HRR/injected heat value). Accordingly, the combustion reaction speed was examined in relation to different EGR volume fractions, and the results are shown in Fig. 17. The internal and external EGR volume fractions do not show a strong effect on suppressing the combustion reaction speed until the former is increased to 20% (interval O) and the latter to 15% (interval P). Increasing the EGR volume fraction further, however, does have an effect on restraining the combustion reaction speed.

The relationship between the EGR mass and the combustion reaction speed was then examined, and the results are shown in Fig. 18. For both internal and external EGR, the combustion reaction speed does not change up to a gas mass of approximately 30 mg (region Q). A restraining effect on the combustion reaction speed is seen at nearly the same time (region R) for both EGR types. It is inferred from these results that under a condition of a constant equivalence ratio the EGR mass, not the EGR volume fraction, governs the suppression of the combustion reaction speed. In other words, external EGR with its larger mass per unit volume is more effective than internal EGR for suppressing the combustion reaction speed. The experimental results in this study also showed that external EGR was more effective than internal EGR. It is thought that the use of an EGR cooling system would increase the restraining effect further.

Figure 19 shows the indicated thermal efficiency $\eta_i$ and Fig. 20 shows the indicated mean effective pressure $P_{mi}$ as a function of the EGR volume fraction for both internal and external EGR. The results in these two figures indicate that both $\eta_i$ and $P_{mi}$ decline as the internal EGR volume fraction is increased. In contrast, the indicated thermal efficiency is improved as the external EGR volume fraction is increased, which is attributed largely to the retarding of the ignition timing and suppression of the combustion reaction speed. However, because of the reduction of the injected heat value, the indicated mean effective pressure increases only slightly.

6. CONCLUSIONS

In this study, a 2-stroke test engine was operated on n-heptane under a condition of a constant equivalence ratio in relation to the fresh air and varying volume fractions of internal and external EGR gas. The experimental results made the following points clear:
1. It was found that the absorbance waveform can indicate changes in the concentration of intermediate combustion products and that their rate of production can be known from the rate of change in absorbance.

2. The absorbance waveform and rate of change in absorbance can indicate changes in low-temperature oxidation reactions due to the application of EGR.

3. Light emission due to the production of HCHO in a cool flame is influenced by the in-cylinder temperature, gas concentration and also the intensity of the HCHO production reactions.

4. Internal EGR has a dominant effect on changing the state of combustion by raising the in-cylinder temperature at the onset of compression.

5. External EGR has a dominant effect on changing the state of combustion by varying the gas composition.

6. The EGR mass, rather than its volume fraction, has a dominant effect on suppressing the combustion reaction speed.

7. The use of an EGR cooling system would probably be effective in strengthening the effect on suppressing the combustion reaction speed.

8. Increasing the external EGR volume fraction was shown to improve indicated thermal efficiency and indicated mean effective pressure.

REFERENCES


CONTACT
For further information, please contact the authors at the following e-mail addresses:

Hiroki Kasuya
E-mail: m0506008tw@edu.cst.nihon-u.ac.jp

Akira Iijima
E-mail: iijima@mech.cst.nihon-u.ac.jp

Hideo Shoji, Professor
Email: shoji@mech.cst.nihon-u.ac.jp