

A Study of HCCI Combustion using Spectroscopic Techniques and Chemical Kinetic Simulations

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ABSTRACT

This study was conducted to investigate the influence of low-temperature reactions on the Homogeneous Charge Compression Ignition (HCCI) combustion process. Specifically, an investigation was made of the effect of the residual gas condition on low-temperature reactions, autoignition and the subsequent state of combustion following ignition. Light emission and absorption spectroscopic measurements were made in the combustion chamber in order to investigate low-temperature reactions in detail. In addition, chemical kinetic simulations were performed to validate the experimental results and to analyze the elemental reaction process. The results made clear the formation behavior of the chemical species produced during low-temperature HCCI reactions.

INTRODUCTION

There are strong demands today for improvement of the efficiency of internal combustion engines so as to reduce fuel consumption, against a backdrop of global warming, depletion of petroleum resources and other concerns. At the same time, it is also necessary to reduce harmful exhaust gases in order to address air pollution problems. In short, high-efficiency, clean engines are being demanded. Gasoline engines now achieve clean exhaust gas than diesel engine through the use of electronically controlled fuel injection systems and three-way catalysts [1], but they are still inferior to diesel engines with respect to thermal efficiency. Although diesel engines provide outstanding thermal efficiency, they have the drawback that it is difficult to simultaneously reduce emissions of nitrogen oxides (NO_x) and particulate matter (PM). Against this backdrop, Homogeneous Charge Compression Ignition (HCCI) engines [2-9] have attracted much interest because they achieve thermal efficiency equal to that of diesel engines while simultaneously reducing NO_x and PM emissions.

In gasoline-fueled HCCI engines, it is necessary to autoignite the gasoline fuel that does not ignite easily on account of its high octane number. One promising way of accomplishing that is to induce and control ignition by applying high-temperature residual gas [10-13] using negative valve overlap or a variable valve mechanism. For diesel-based HCCI engines, methods

are being researched for promoting premixing of the charge through early injection [14-15] or by extending the ignition delay time without advancing the fuel injection timing [16-17]. However, chemical reactions have a stronger effect on HCCI combustion compared with traditional combustion systems. Therefore, in order better to comprehend and control HCCI ignition and combustion, it is necessary to have a more detailed understanding of the characteristics of these processes.

In this study, the characteristics of HCCI combustion were investigated in detail under the application of residual gas using both experimental and computational methods. The former included spectroscopic measurements of light emission and absorption during HCCI combustion and observations of visualized images of in-cylinder conditions. The latter involved analyses of chemical reactions based on chemical kinetic simulations.

EXPERIMENTAL EQUIPMENT AND PROCEDURE

The test equipment used in this study is shown schematically in Fig.1, and the specifications of the test engine are given in Table 1.

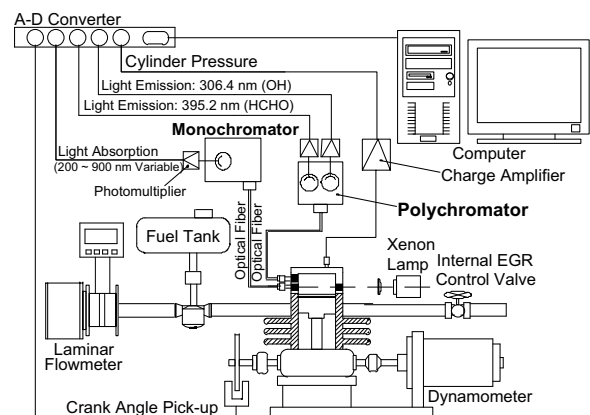


Fig. 1 Configuration of test equipment

Table 1 Specifications of test engine

2-stroke Air Cooled SI Engine	
Scavenging Type	Schnürle
Bore × Stroke	72 × 60 mm
Displacement	244 cm ³
Effective Compression Ratio (ϵ_e)	10.7 / 12: 1 / 5.7: 1
Test Fuel	heptane (RON)

A two-stroke engine with a combustion chamber that allowed large degrees of measurement freedom was used in the experiments. Two-stage ignition accompanied by a cool flame, which is a characteristic feature of four-stroke HCCI combustion, is observed in this test engine when a low-octane fuel is autoignited by compression under a condition of a high delivery ratio (low residual condition). This indicates that four-stroke HCCI combustion can be simulated with this engine [18]. Furthermore, residual gas in the form of internal exhaust gas recirculation (EGR) can be intentionally applied by exhaust port throttling.

The following experiments were conducted in this study:

<Analysis of low-temperature reactions and autoignition behavior>

- Measurement of absorption spectra
- Simultaneous measurement of light absorption and emission

<Observation of conditions for hot flame development>

- 2D combustion image measurement by in-cylinder visualization

Figure 2 shows a schematic diagram of the cylinder head and measurement equipment used in measuring absorption spectra. Light from an external light source was introduced into the cylinder through window A and the transmitted light was extracted from window B. The extracted light was then introduced into a variable-wavelength spectroscopy (Monochromator) and a photomultiplier to obtain the transmitted light intensity. Absorption spectra were obtained by measuring the transmitted light at each wavelength of interest. In this study, absorption was investigated from the ultraviolet to the visible light region of the spectrum in order to detect absorption by intermediate combustion products generated in low-temperature reactions, such as formaldehyde (HCHO). A xenon lamp was used as the external light source because it is capable of providing a continuous spectrum of stable intensity over a wide range of wavelength from the ultraviolet to the infrared region.

Light absorbance (A) is defined as equation (1), where E_0 is the transmitted light intensity at bottom dead center and E is the transmitted light intensity at any arbitrary crank angle.

$$A = \frac{E_0 - E}{E_0} = 1 - \frac{E}{E_0} \quad (1)$$

A schematic diagram of the cylinder head and measurement equipment used to obtain simultaneous measurements of light emission and absorption is shown in Fig. 3. While absorption of 293.1 nm corresponding to the light absorption wavelength of formaldehyde (HCHO) [19] was measured via the C-D

window system, light emission in the combustion chamber was extracted through window E and introduced into a multi-wavelength spectroscopy (Polychromator) and a photomultiplier to measure the light emission intensity at two specific wavelengths. One wavelength was 395.2 nm, corresponding to the light emission wavelength of HCHO that forms during low-temperature reactions [19]. The other was 306.4 nm, corresponding to the light emission wavelength of the OH radical [19] that plays a key role in the progress of combustion reactions.

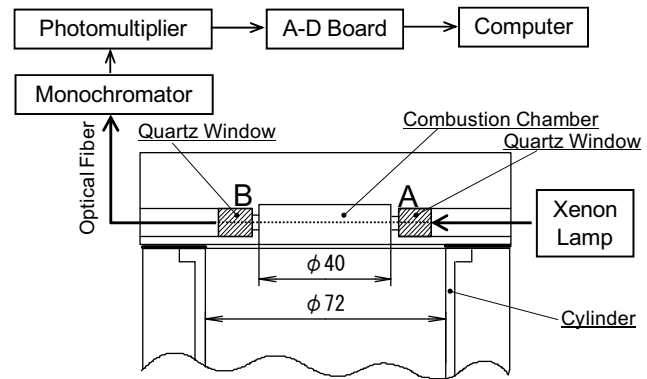


Fig. 2 Schematic diagram of cylinder head for light absorption measurement ($\epsilon = 10: 1$)

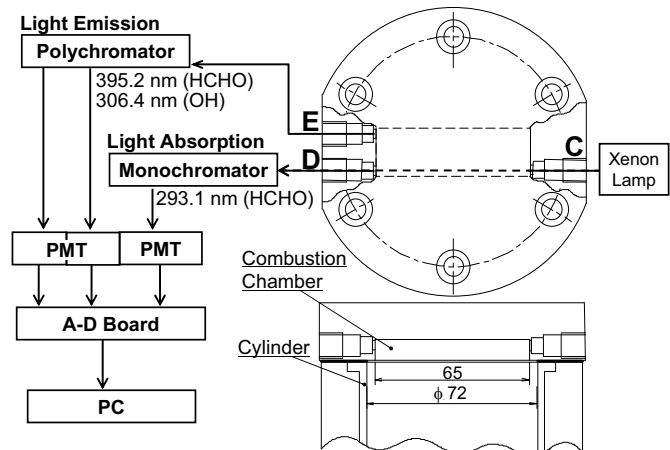


Fig. 3 Schematic diagram of cylinder head for simultaneous measurement of light absorption and emission ($\epsilon = 12: 1$)

A schematic diagram of the optically accessible engine used for flame visualization is shown in Fig. 4. A quartz window was provided in the cylinder head to allow combustion to be visualized across the entire cylinder bore. Color combustion images were captured with a high-speed video camera. Flame light was extracted through two quartz windows provided on opposite sides of the cylinder, and light emission intensities were measured simultaneously at two wavelengths. One wavelength was 395.2 nm, representative of the blue CO-O glow, and the other was 700 nm, representative of a longer light emission wavelength where red light was emitted. When this cylinder head for flame visualization was used, the effective compression ratio of the engine was $\epsilon = 5.7:1$.

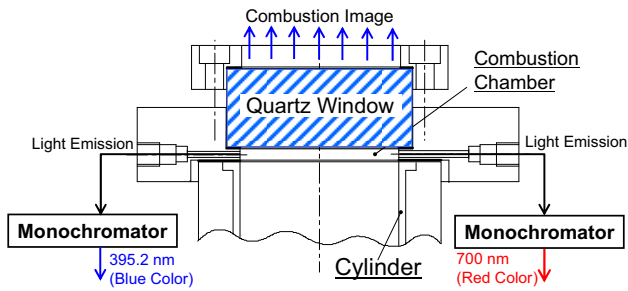


Fig. 4 Schematic diagram of cylinder head for flame visualization ($\epsilon = 5.7: 1$)

DEFINITION OF INTERNAL EGR RATE

Throttling the flow through the internal EGR control valve lowered the delivery ratio and applied internal EGR (residual gas). The internal EGR rate was defined on the assumption that a state of perfect mixing and scavenging existed in the cylinder [1]. Assuming initial operating conditions of an engine speed $N = 1000$ rpm and wide open throttle (WOT), the initial scavenging efficiency (η_{si}) and initial residual gas fraction (γ_i) were calculated from the corrected delivery ratio (L_i) at that time using the following equations.

$$\eta_{si} = 1 - \exp(-L_i)$$

$$\gamma_i = 1 - \eta_{si}$$

The scavenging efficiency (η_s) and residual gas fraction (γ) were then calculated from the corrected delivery ratio (L) when the flow through the internal EGR control valve was throttled.

$$\eta_s = 1 - \exp(-L)$$

$$\gamma = 1 - \eta_s$$

Based on these calculations, the internal EGR rate (γ_{EGR}) was defined as the difference between the residual gas fraction γ when the flow through the internal EGR control valve was throttled and the initial residual gas ratio γ_i . The Internal EGR rate (γ_{EGR}) could be varied intentionally by adjusting the control valve setting and was given by following equation.

$$\gamma_{EGR} = (\gamma - \gamma_i) \times 100 \quad [\%]$$

CALCULATION METHOD

Based on the formation behavior of the chemical species observed in the experimental results, chemical kinetic simulations were run to analyze the chemical reaction mechanisms during the combustion process in more detail.

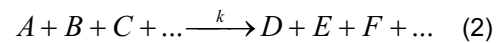
Numerical calculations of elementary reactions were performed using the CHEMKIN 4.0 IC Engine under dimensionless, adiabatic conditions and by applying the same volumetric change as that of the test engine. The reaction mechanism used in the calculations was

developed at the Lawrence Livermore National Laboratory (LLNL) for primary reference fuels (PRF) and included 1,034 chemical species and 4,236 elementary reactions [20-22]. In the calculations involving the application of residual gas, the following assumptions were made concerning the gas temperature and composition.

- The residual gas temperature was assumed to be 900 K.

- The internal EGR composition is assumed to complete combustion composition of the mixture. The components include N_2 , O_2 , CO_2 and H_2O .

Generally, elementary reaction can be described by the equation (2)



where A, B, C, D, E, F,... denote the different species involved in the reaction.

Looking at the production of species D, the reaction rate can be expressed by the equation (3)

$$\frac{d[D]}{dt} = k \cdot [A][B][C] \dots \quad (3)$$

where $[D]$ is the mole concentration of the species D.

And k is the reaction rate coefficient of the reaction which strongly depends and in a nonlinear way on the temperature (Arrhenius law).

$$k = AT^B \exp\left(-\frac{E_a}{RT}\right)$$

where A is the frequency factor, B is the constant number, T is the temperature, E_a is the activation energy of the reaction and R is the gas constant.

A , B , E_a , and R were given by chemical reaction mechanism (i.e. LLNL-PRF reaction mechanism) and thermodynamic properties.

RESULTS AND DISCUSSION

LIGHT ABSORPTION SPECTRA OF HCCI COMBUSTION

Light absorption spectra were investigated to make clear the formation behavior of chemical species and other characteristics during the autoignition process of HCCI combustion. The measurement conditions used are given in Table 2 for cases 1 and 2. The scavenging efficiency (η_s) shown in the table was calculated in each case from the corrected delivery ratio assuming perfect mixing scavenging [1]. The fuel used was n-heptane (0 RON), which is conducive to low-temperature reactions, and the residual gas fraction was changed by applying or not applying

internal EGR. Under this condition, the amount of residual gas increased with a smaller η_s value.

Table 2 Measurement conditions for light absorption spectra

	Operating Mode	Scavenging Efficiency η_s [-]	ε [-]	Qin [J/cycle]	Intake Equivalence Ratio, ϕ [-]	N [rpm]	Fuel
Case 1	Without In-EGR	0.73	10:1	304 ± 5	0.44	1000	n-heptane (0 RON)
Case 2	With In-EGR	0.42			1.04		

The results of the light absorption spectrum analysis are shown in Figs. 5 and 6 for Cases 1 and 2, respectively. From the top, the graphs in each figure show the HRR waveform, the contours of the light absorption spectra in a wavelength range of 200-800 nm, the enlarged contours of the light absorption spectra for the wavelength region of 200-400 nm, and absorbance measured at a wavelength of 290 nm. In the black-and-white contour representations, absorbance increases with a darker color. All of the waveforms indicate measured data averaged for ten cycles under identical conditions.

The light absorption spectra in Fig. 5 for Case 1 with a small amount of residual gas show evidence of strong absorbance between roughly 260 nm and 320 nm in the ultraviolet region (denoted by α) simultaneous (LTR_{peak}) with the development of a cool flame.

Presumably, this mainly represents light absorption by HCHO [19] produced accompanying the cool-flame reactions [23-24]. The behavior of the absorbance waveform at 290 nm clearly shows the occurrence of strong light absorption concomitant with the cool-flame reactions, followed by a gradually rising absorbance slope accompanying the degeneration of heat release from the cool flame. Absorbance then declines sharply concomitant with the occurrence of the hot flame (HTR_{peak}). This decrease likely indicates the consumption of HCHO that was produced accompanying autoignition. The results also show that light absorption continues at 310 nm after ignition occurs, which probably represents absorption by OH that was rapidly produced accompanying ignition. In other words, the results at 310 nm are ascribed primarily to HCHO before ignition and to OH after ignition.

The light absorption spectra in Fig. 6 for Case 2 with a large quantity of residual gas show a gradual rise (denoted as β) in absorbance during the cool-flame reactions. Subsequently, absorbance increases until just before ignition and then decreases sharply concomitant with ignition (region denoted as γ in the figure). The interval (τ) from the occurrence of the cool flame to autoignition is longer than in Case 1. This result indicates that the application of residual gas moderates the cool-flame reactions and lengthens the subsequent interval to autoignition. The foregoing results imply that the activity level of the low-temperature reactions prior to ignition can be ascertained by investigating absorbance behavior in a wavelength range from 260 nm to 320 nm.

The foregoing results have made it clear that strong light absorption takes place in the ultraviolet region at

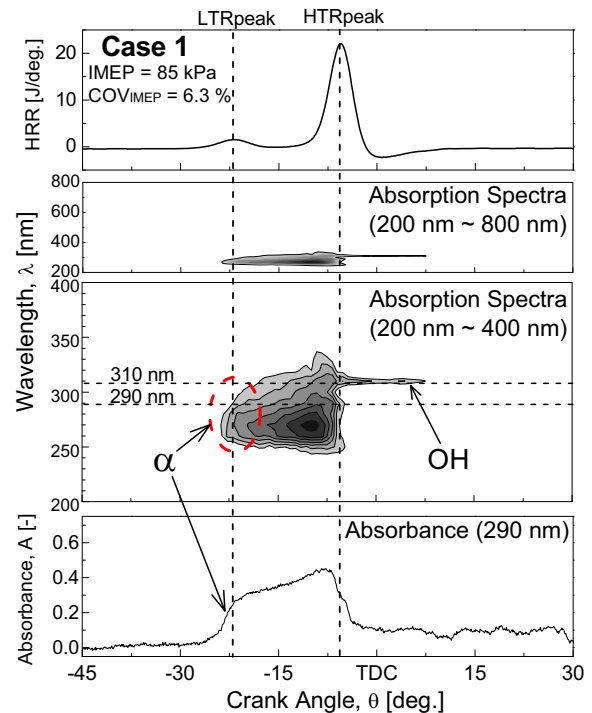


Fig. 5 Light absorption spectra for HCCI combustion (Case 1)

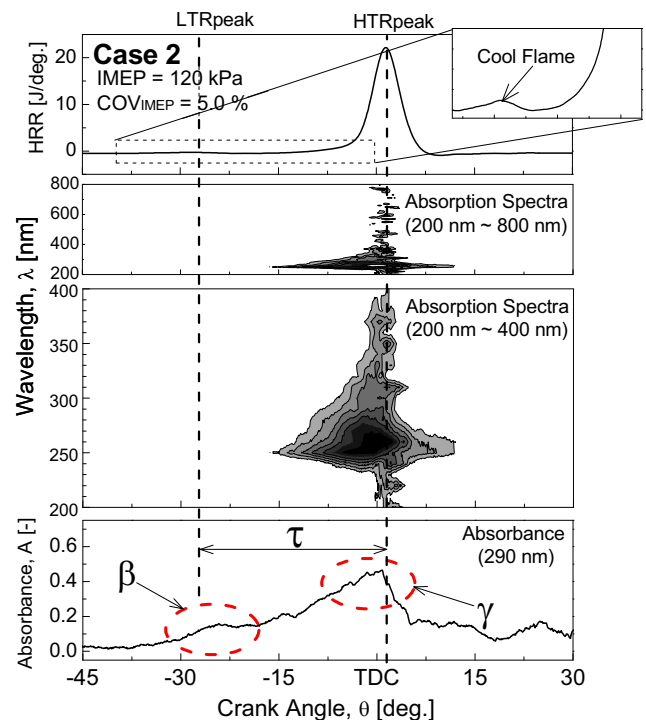


Fig. 6 Light absorption spectra for HCCI combustion (Case 2)

the time a cool flame occurs. In addition, increasing the residual gas fraction weakens the level of light absorption in the ultraviolet region when a cool flame occurs (regions β Fig. 6). However, even under conditions where light absorption decreases when a cool flame occurs, absorbance increases prior to the development of the hot flame (regions γ in Fig. 6), and the peak absorbance value is not so different from that seen for the conditions where a cool flame tends to occur. In other words, the magnitude of the