UV–visible light absorption by hydroxyl and formaldehyde and knocking combustion in a DME-HCCI engine

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ABSTRACT

Experiments were conducted in a compression–expansion test engine to investigate the combustion characteristics in a homogeneous charge compression ignition (HCCI) engine fuelled with dimethyl ether. Two types of analyses were performed. In the first, ultraviolet–visible (UV–Vis) light absorbance was investigated to identify the formation behaviour of HCHO and OH during HCCI combustion. In the second, knocking combustion was investigated by analysing the spatially integrated flame luminosity and in-cylinder pressure oscillations. The time-resolved HCHO and OH profiles at different equivalence ratios showed that HCHO absorbance increased in the low-temperature reaction (LTR) and thermal-preparation regions and gradually decreased as the combustion approached the high-temperature reaction (HTR) region. The in-cylinder temperature in the LTR region had little effect on the rate of the maximum pressure rise, and this did not change much at different equivalence ratios. The results demonstrated that there was a marked difference between the intensity of the flame emissions of non-knocking and knocking events. The time-resolved integrated absorbance spectra of HCHO with peaks at 328, 340, and 354 nm that occurred before the OH peaks appeared suggested that when a certain threshold ratio of $(dP/d\theta_{\mathrm{LTR}})/(dP/d\theta_{\mathrm{HTR}})$ was reached, the amount of HCHO decreased due to reactions in the thermal-preparation region while the tendency to knock increased.

1. Introduction

Homogeneous charge compression ignition (HCCI) engines have been drawing the attention of many researchers due to their high efficiency and lower nitrogen oxide (NOx) and particulate matter (PM) emissions. Most recent studies on HCCI have focused on four-stroke engines [1,2]. In recent years, research on HCCI engine fuelled with dimethyl ether (DME) has drawn the attention of experts in engine technology, because DME fuel exhibits very strong low-temperature kinetic reactions. DME is suitable for compression ignition engines and is considered a promising alternative fuel with the potential to solve air-pollution problems caused by soot and NOx [3]. Therefore, a study of an HCCI engine fuelled with DME may provide useful information on the low-temperature kinetic reactions for HCCI operation with other fuels. The oxidation of DME has been examined in a number of studies and recent research has led to the development of detailed and reduced chemical kinetics models of DME combustion [4–6].

To understand the DME oxidation mechanism in an HCCI engine, an experimental study of DME combustion must be conducted. One effective way to study the DME reaction mechanisms is to use a spectrum analysis to determine the major active species during combustion process [7,8]. For example, a number of combustion studies have examined HCHO absorption in a constant volume vessel or a reactor [9,10]. A few studies have examined HCHO and OH formation at normal engine conditions [11,12]. Understanding of HCHO and OH formation process can help resolve problems related to knocking combustion. In internal combustion (IC) engines, engine knock is related to HCHO in the hot spots (exothermic centres) of the slow oxidation process prior to autoignition [13,14]. HCHO is an important intermediate species in the cool flames preceding the main combustion. It has been shown that the local HCHO concentration dramatically decreases in locations where the peak heat release rates appear [15].

Therefore, the objective of this study was to investigate the HCHO and OH species formation during combustion in an HCCI engine fuelled with DME. Absorption spectroscopy was applied to determine the light absorption of HCHO and OH during the DME combustion process, which includes low-temperature oxidation and high-temperature ignition. The major intent was to characterise the time-resolved spectra of HCHO and OH species as representative

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Nomenclature

HCCI	homogeneous charge compression ignition
DME	dimethyl ether
CA deg.	crank angle degree
IVC	intake valve closure
LTR	low-temperature reaction
HTR	high-temperature reaction
$ROHR_{LTR\_START}$	peak value of $d^2(ROHR)/d\theta^2$ before the start of the LTR (J/deg.)
$ROHR_{LTR\_PEAK}$	peak value of the heat release rate in the LTR region (J/deg.)
$ROHR_{HTR\_START}$	peak value of $d^2(ROHR)/d\theta^2$ before the start of the HTR (J/deg.)
$ROHR_{HTR\_PEAK}$	peak value of the heat release rate in the HTR region (J/deg.)

T_{LTR_START}	low-temperature-reaction starting temperature (K)
T_{LTR_PEAK}	temperature at $ROHR_{LTR\_PEAK}$ (K)
T_{HTR_START}	high-temperature-reaction starting temperature (K)
T_{HTR_PEAK}	temperature at $ROHR_{HTR\_PEAK}$ (K)
P_{LTR_START}	low-temperature-reaction starting pressure (MPa)
P_{LTR_PEAK}	pressure at $ROHR_{LTR\_PEAK}$ (MPa)
P_{HTR_START}	high-temperature-reaction starting pressure (MPa)
P_{HTR_PEAK}	pressure at $ROHR_{HTR\_PEAK}$ (MPa)
NTC	negative temperature coefficient
SIFL	spatially integrated flame luminosity
$d(SIFL)/d\theta$	rate of the maximum flame luminosity change
RI	ringing intensity (MW/m^2)

indicators of low-temperature oxidation and high-temperature ignition, respectively. Knocking combustion during HCCI was investigated by estimating the knock intensity derived from in-cylinder pressure oscillations and from the rate of change of the flame luminosity derived from spatial integration of the flame luminosity.

2. Experimental setup and procedure

2.1. Test engine

HCCI fuelled with DME was studied in an optical compression–expansion test engine with a single cylinder and a compression ratio of 9.0. Fig. 1 shows a schematic diagram of the experimental setup (A) and an optical head (B), and Table 1 summarises the test engine specifications (A) and experimental conditions (B). The engine crank was driven externally by a 2000 W induction motor and made to rotate at a fixed rpm. The DME was premixed with gas at a ratio of 20% oxygen to 80% argon at molar proportions equivalent to ϕ = 0.26, 0.28, 0.30, and 0.34. Argon was used instead of nitrogen to increase the in-cylinder temperature at the end of compression by decreasing the heat capacity of the in-cylinder gas–fuel mixture and to initiate HCCI combustion at a compression ratio that was significantly lower than those usually used in conventional HCCI engines. The DME–O_2–Ar fuel mixture was supplied to the mixture tank, where it was heated to the required temperature and maintained at the required pressure. During operation, the intake valve remained open, and the fuel mixture was sucked into the cylinder and pushed back into the mixture tank. When the thermocouple reading was stabilised, the intake valve was closed at around bottom dead centre (BDC), and the fuel mixture was compressed, autoignited, and combusted. Changes in the gas pressure were measured using a KISTLER 6052B pressure transducer during the compression and expansion strokes. Combustion inside the cylinder was visualised with a MEMRECAM GX-1 Nac Image Technology high-speed camera. The top of the piston was fitted with a quartz window with visualisation region diameter of 52 mm. This window permitted a view of the chamber cross-section to observe the flame emissions during combustion.

The compressed gas temperature range accessible in the compression–expansion test engine was relevant to combustion in HCCI and related engines, but the in-cylinder pressure at TDC was somewhat lower because the initial pressure was less than one atmosphere. Thus, good temporal resolution was more easily achieved, although at the expense of longer ignition delays than those encountered in practical applications. The volumetric heat release in the final stage of ignition was also lower as a result of the reduced gas densities. However, pressure oscillations were still observed, even with very lean mixtures. The gaseous charge admitted to the cylinder of the compression–expansion test engine was premixed at the molecular level. Therefore, unlike engines with a normal induction system for evaporating liquid fuels, the problem of distinguishing the effect of the initial spatial composition variations from the spatial temperature field variations did not arise.

2.2. Light absorbance acquisition system

The UV–Vis spectral absorbance was determined by applying the Beer–Lambert law to the measured spectral transmission:

$$A(\lambda) = \log_{10}\left[\frac{I_0(\lambda)}{I(\lambda)}\right] = \varepsilon cL, \tag{1}$$

where $A(\lambda)$ is the spectral absorbance, $I_0(\lambda)$ is the intensity through an air-filled cylinder, $I(\lambda)$ is the intensity through a DME–O_2–Ar-filled cylinder, ε, c and L are molar absorption coefficient, molar concentration, and measurement length, respectively. A schematic diagram of the light absorbance acquisition setup is shown in Fig. 1B. The combustion chamber was illuminated with light from a xenon lamp, and the transmitted light was introduced through an optical fibre cable into the spectrometer (Andor Technology, SR-163), which was equipped with an intensified charge-coupled device (CCD) (Andor Technology, DK720-18F-04). The spectral absorbance measurements were made under engine conditions for the $\widetilde{A}^1A_2 \leftarrow \widetilde{X}^1A_1$ formaldehyde system in the region of 260–400 nm.

Fig. 2A shows samples of high-speed camera images of the DME–O_2–Ar mixture combustion in the high-temperature reaction (HTR) region under HCCI conditions, along with the pressure history and the rate of heat release (ROHR) obtained simultaneously with the flame images. This figure indicates that the HCCI combustion process could be divided into two consecutive parts: a low-temperature reaction (LTR) region, and a main heat release, HTR region; both parts were visible on the pressure trace and the rate of heat release curve. The LTR region was characterised by low oxidation of DME. The main region was characterised by distributed reactions throughout the combustion chamber. The distributed reactions appeared to progress inhomogeneously. This effect was observed from the instantaneous images of combustion in the HTR region. The inhomogeneity was due to temperature and concentration fluctuations. Combustion appeared as a blue flame; a luminescent flame from soot was not observed.

2.3. Method of defining ignition timing

Fig. 2B shows the definitions of various crank-angle timings representing the LTR and HTR. This figure is based on the results of