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Ignition properties of lean DME/H$_2$ mixtures at low temperatures and elevated pressures

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ABSTRACT

Ignition delays of lean dimethyl ether (DME)/hydrogen mixtures with hydrogen mole fraction ranging from 0 to 85% were measured using a rapid compression machine with equivalence ratios from 0.3 to 0.5, temperatures from 621 to 852 K and pressures from 7 to 22 bar. Numerical analysis was performed based on the NUI Aramco Mech 2.0 and, in general, good agreement between measurements and predictions was demonstrated. Both measurements and predictions show that H$_2$ addition increases the ignition delay of DME/H$_2$ mixtures non-linearly. Moreover, the effect of H$_2$ addition on ignition delay becomes more pronounced at H$_2$ mole fraction above 70% and lower pressure. The dilution and chemical effects of H$_2$ addition were quantified, and the dilution effect decreases whereas the chemical effect increases with the increase of H$_2$ mole fraction. It is also found that DME/H$_2$ mixtures show a three-stage heat release behavior at very lean condition (φ = 0.3), namely, a low temperature heat release (LTHR) stage followed by two high temperature heat release (HTHR) stages. The first- and second-stage HTHR are caused by the conversion of HCHO to CO and the production of final reaction products CO$_2$ and H$_2$O respectively. Overall, DME is mainly consumed during the LTHR and first-stage HTHR whereas H$_2$ is mainly consumed during the second-stage HTHR. The two-stage HTHR behavior of DME/H$_2$ mixtures occurs when H$_2$ and HCHO produced during DME's LTHR stage are present in a proper proportion prior to high-temperature ignition and the temperature after LTHR has reached a proper level.

1. Introduction

The homogeneous charge compression ignition (HCCI) has been studied extensively because of its extremely high thermal efficiency and low emissions compared to conventional combustion mode [1]. However, the ignition timing of HCCI combustion is difficult to control and the operational range is limited [2,3]. The commonly known reason is that the ignition and combustion process of HCCI are fully dependent on fuel chemical kinetics. An effective method to resolve this issue is the use of blending fuels that have different ignition properties [4,5]. DME as a promising alternative fuel has a high cetane number and is easily ignited at relatively low temperatures [6]. Meanwhile, the high oxygen content and absence of C−C bond enable DME to achieve an almost smokeless effect during HCCI combustion. Nevertheless, DME engines are prone to knock at high loads [7]. Hydrogen, another well-known

clean alternative fuel, has been regarded as an excellent anti-knock additive [8]. Therefore, from the perspective of ignition control and load expansion, a HCCI engine fueled with DME/H$_2$ mixtures has been proposed [9].

Based on the above considerations, research on internal combustion engines has been conducted. Shudo et al. [10] studied the ignition characteristic of DME/H$_2$ mixtures in a HCCI engine and they found that adding 60% H$_2$ to DME could retard the ignition timing by 15 crank angle degrees and extend the equivalence ratio from 0.32 to 0.37. Liu et al. [11] numerically studied the effect of H$_2$ addition to DME/CH$_4$ on a dual fuel reactivity controlled compression ignition (RCCI) engine and they found that the ignition timing was advanced and the peak cylinder pressure was increased by adding H$_2$. In the work by Jeon et al. [12], the performance and emission of DME-H$_2$ premixed charge compression ignition (PCCI) combustion were compared to those of

DME PCCI combustion on a single-cylinder engine. Their results showed that CO, CO$_2$ and HC emissions decreased as the hydrogen mole fraction increased. Numerical studies from Zheng et al. [13] showed that the addition of reformed gases (CO and H$_2$) could delay the ignition timing and broaden the load range of DME HCCI engine, and they concluded that the ignition time was mainly dominated by H$_2$.

Although DME/H$_2$ mixtures exhibit a better engine performance compared to pure DME, further fundamental study is needed to understand its acting mechanism on ignition and combustion properties. DME/H$_2$ mixtures have been investigated including experiments and simulations such as oxidation [14,15], laminar flame speed [16,17] and flame [18–20] extensively. The ignition delay, which is an important parameter to indicate the combustion mechanism, is also focused. It is critical data to develop, validate and refine the chemical kinetic models. Pan et al. conducted a shock tube experiment to measure the ignition delay of DME/H$_2$ mixtures diluted by 80% argon (hydrogen mole fraction ranging from 0 to 100%) at equivalence ratios of 0.5, 1, and 2 and at pressures of 1.2 and 10 atm over a wide temperature range (900–1700 K) [21]. Their results demonstrated three ignition regimes depending on hydrogen fraction and hydrogen addition non-linearly decreased the ignition delay. They also found that the dependence of ignition delay on pressure and equivalence ratio changed at different hydrogen mole fractions [22]. Different from high-temperature and low-pressure conditions, numerical studies [23–25] showed that the ignition delay of DME/H$_2$ mixtures increased with increasing the hydrogen mole fraction at low temperatures and high pressures. Recently, Shi et al. [26] measured the ignition delay of stoichiometric DME/H$_2$ mixtures at high dilution and hydrogen mole fraction less than 60% in a rapid compression machine (RCM) and their experimental data showed that H$_2$ addition increased the ignition delay, especially in the negative temperature coefficient (NTC) region.

Additionally, Iijima and Komatsu et al. [27,28] conducted experimental and numerical studies in a supercharged HCCI engine; their results indicated that the DME/CH$_4$ mixtures exhibited three-stage heat release behavior depending on fuel mixing ratio, intake air pressure and equivalence ratio, and adding 30% CH$_4$ to DME reduced the peak HRR (heat release rate) by approximately 20%. Other studies have shown that pure DME also exhibited three-stage ignition and heat release characteristics under lean and stoichiometric conditions [29–31]. Recently, Hu et al. [32] numerically confirmed that DME with 30%, 50% of hydrogen in a HCCI engine showed the three-stage heat release behavior at the initial temperature of 380 K, initial pressure of 0.1 Mpa and very lean conditions (φ = 0.3), while the mechanism of this phenomenon was not explained. And, this three-stage heat release characteristic could reduce combustion roughness by lowering the peak HRR and the rate of pressure rise.

From above, the high-temperature ignition properties of DME/H$_2$ mixtures have been fully experimentally and numerically investigated. However, the ignition delay data of lean DME/H$_2$ mixtures at low temperatures and elevated pressures are still meager and its ignition properties needs to be further understood. Meanwhile, the mechanism of three-stage heat release for DME/H$_2$ mixtures has not been clarified in previous works so far.

Recognizing the gap, we extend the investigation of DME/H$_2$ mixtures to wider pressures (7–22 bar) and hydrogen blending ratios (0–85%) at fuel-lean (φ = 0.3–0.5) conditions on a RCM in the current study. Moreover, all tested conditions are fuel/air mixtures instead of diluted ones, which is more close to the real engine conditions. Furthermore, the mechanism of three-stage ignition and heat release behavior of DME/H$_2$ mixtures under some lean-fuel conditions is analyzed. In addition, ignition data provided at low temperatures and elevated pressures are valuable to further validate and refine the DME kinetic mechanisms [33–40].

2. Experimental setup and procedure

Experiments were conducted on the RCM of Beijing University of Technology, a detailed description of which and results of studies characterizing its performance were described elsewhere [41]. The RCM is driven pneumatically and controlled by a hydraulic braking system. The driver cylinder and reactor cylinder has internal bores of 200 mm and 50 mm respectively. The piston stroke and reactor cylinder volume can be changed by adjusting the number of stroke spacers and clearance spacers, respectively, with compression ratio varying in the range of 8.42–16.9. The total compression time in the experiments is about 20–30 ms depending on compression ratio and driving gas pressure chosen, with most of the rapid rise in pressure and temperature occurring in less than 3 ms before the end of compression; therefore, heat losses during compression are small. The reactor cylinder is equipped with a rapid-response dynamic pressure transducer (Kistler 6125C) to measure the pressure during compression and any post-compression event including ignition. Additionally, a static pressure transducer and a K-type thermocouple are installed to measure the initial pressure and initial temperature, respectively. Both reactor cylinder and premix tank along with connecting lines have a provision for heating up to 400 K. Targeted compressed pressure (P_c) and compressed temperature (T_c) at the top dead center (TDC) are achieved by varying the compression ratio (ε), initial pressure (P_0) and initial temperature (T_0). As used in many RCMs [42–47], a specifically designed creviced piston is used to suppress the roll-up vortex and ensure homogeneous conditions in the reactor cylinder. T_c is calculated from the P_0, T_0, P_c and reactant composition, assuming adiabatic compression and frozen chemistry. They are conducted by using Gaseq [48], which uses the temperature dependence of specific heat ratio, γ, according to the equation:

$$\int_{T_0}^{T_c} \frac{\gamma(T)}{\gamma(T)-1} \frac{dT}{T} = \ln\left(\frac{P_c}{P_0}\right) \tag{1}$$

The schematic diagram of the RCM is shown in Fig. 1.

The purities of the gases used in this study were as follows: DME (99.5%), hydrogen (99.999%), oxygen (99.999%), and nitrogen (99.999%). The gas mixtures were prepared in a premix tank fitted with magnetic stirrer. The connecting lines and premix tank were evacuated to 1 Pa before the mixture is prepared. The gases were then added to the premix tank by the method of partial pressure before heating them to desired initial temperature. Finally, the mixture was stirred for at least 30 min and left to homogenize overnight. The experimental conditions used in this study are presented in Table 1, where the N$_2$/O$_2$ ratio is fixed at 4. R_{H_2} is defined as the mole fraction of H$_2$ in the fuel mixture, and is expressed as:

$$R_{H_2} = n_{H_2}/(n_{H_2} + n_{DME}) \tag{2}$$

Fig. 2 shows the typical pressure profiles of DME/H$_2$ mixtures along with the definitions of the first-stage ignition delay (τ_1) and the total ignition delay (τ) at T_c = 714 K, P_c = 12 bar and φ = 0.5. The first-stage ignition is closely related to the DME low-temperature oxidation. Specifically, the ignition delays (τ_1, τ) are defined as the time between the end of compression, where the pressure peaks at t = 0, and the maximum in the rate of pressure rise at ignition.

Each condition was repeated no less than three times to ensure the repeatability of the experiments, and the pressure profile close to the mean was chosen as the representative pressure profile for reporting the ignition delay. Fig. 3 shows the results from three measurements conducted under the same condition. This RCM has high repeatability and the standard deviation of ignition delay is less than 10% of the mean. There is an uncertainty in the reported ignition delay mainly owing to the uncertainty associated with pressure measurements related to the accuracy of initial pressure and compressed pressure, initial temperature measurements and compression process. According to the