

High-Speed Observation and Modeling of Dimethyl Ether Spray Combustion at Engine-Like Conditions

Yuta Mitsugi, Daiki Wakabayashi, Kotaro Tanaka, and Mitsuru Konno
Ibaraki University

ABSTRACT

Dimethyl Ether (DME) is one of the major candidates for the alternative fuel for compression ignition (CI) engines. However, DME spray combustion characteristics are not well understood. There is no spray model validated against spray experiments at high-temperature and high-pressure relevant to combustion chambers of engines. DME has a lower viscosity and lower volumetric modulus of elasticity. It is difficult to increase injection pressure. The injection pressure remains low at 60 MPa even in the latest DME engine. To improve engine performance and reduce emissions from DME engines, establishing the DME spray model applicable to numerical engine simulation is required.

In this study, high-speed observation of DME sprays at injection pressures up to 120 MPa with a latest common rail DME injection system was conducted in a constant volume combustion vessel, under ambient temperature and pressure of 6 MPa-920 K. The spray penetration, evaporation, liquid length and ignition delay were investigated and compared with those of diesel sprays. Based on the observed results, the spray model of DME was developed. A reduced chemical kinetic model for the oxidation of DME, that included 27 species and 52 reactions, was made and coupled with the spray model. Calculated results showed good overall agreement with experimental data, such as spray tip penetration, faster evaporation, and short liquid length. Ignition delay time was slightly longer compared with experiment. Using this model, engine simulation was performed. The results showed a reasonable agreement with the experiments.

CITATION: Mitsugi, Y., Wakabayashi, D., Tanaka, K., and Konno, M., "High-Speed Observation and Modeling of Dimethyl Ether Spray Combustion at Engine-Like Conditions," *SAE Int. J. Engines* 9(1):2016, doi:10.4271/2015-01-1927.

INTRODUCTION

Dimethyl Ether (DME : CH_3OCH_3) is a clean alternative fuel for Compression Ignition (CI) engines. DME creates no soot in combustion, because it has an oxygen atom and no carbon-carbon bonds in the molecule. DME features good auto ignition characteristics, despite its low-molecular weight due to the active low-temperature oxidation mechanisms. The cetane number of DME is as high or higher than that of diesel fuel.

Studies on DME as CI engine fuel started in 1990s, when Haldor Topsoe developed a low-cost mass production process [1]. In 1995, Sorenson applied DME to a conventional small diesel engine with a simple modification [2]. Kajitani et al. had succeeded in the operation of DME fueled CI engine, and showed good performance and cleaner exhaust emission characteristics [3]. In 2001, Gill et al. showed that DME can be applied to a heavy duty CI engine with a suitable injection system [4]. Hansen et al. demonstrated the feasibility of DME fueled city bus through field tests [5]. Konno et al. observed DME spray combustion and intermediate chemical products in an actual DME fueled engine, and revealed the mixture formation and the combustion process [6]. Goto and Oguma developed a medium duty DME truck with a driving range of 500 km in one fueling and

with fuel efficiency of 5.75 km/l [7, 8]. They reported that there was no inferiority in performance of DME trucks compared with conventional diesel engine-powered trucks.

Recently, Isuzu Central Research Institute has developed medium duty DME trucks equipped with a common rail injection system [9]. The exhaust emissions and the fuel consumption were improved by optimizing the compression ratio and EGR rate. They reported that a 100,000 km road test was successfully conducted. Practical road tests are currently being conducted by two transportation companies in Japan.

Studies on chemical kinetic mechanisms for DME oxidation began with the works of Dagaut [10] and K. Sato et al. [11] in 1996. These two chemical mechanisms were made with an emphasis on high-temperature region. Based on the mechanisms of H.J. Curran et al. extended it to low-temperature range and determined the overall reaction scheme for DME oxidation [12]. The scheme showed the capability of predicting both low and high-temperature oxidation of DME. Zhao et al. added oxidation paths through formic acid and methanol [13]. The elementary reaction model of Zhao et al. showed qualitatively good agreement with the experimental results of a mild compression machine over a range from Negative-Temperature-

Coefficient (NTC) region to high-temperature region, though it has a tendency to predict longer ignition delay times [14]. Recently, Burke et al. developed new chemical kinetic models [24] capable of predicting the DME combustion in common combustion environments of CI engines.

Cung et al. performed the simulation of DME spray to predict NO and soot formation under engine relevant conditions using Zhao's mechanism [15]. The paper provided valuable information about the effects of ambient temperature, EGR, and injection pressure on DME spray combustion, however, the spray model was not experimentally validated.

The authors have developed a reduced kinetic mechanism with 26 chemical species and 37 chemical reactions, on the basis of Zhao's scheme and applied it to model DME spray combustion [16]. The calculated ignition delay times were slightly longer than those observed in a constant volume vessel, though agreed well with the times calculated by Zhao's full scheme.

It is necessary to understand spray combustion characteristics and to establish a reliable model because they are essential for development of DME CI engines. However, the sufficiently-reliable model of DME spray combustion has not been established.

One of the major reasons is that there are few observation results for validating the models under the pressure and temperature of engine-relevant conditions.

In this study, we conducted high speed observation of DME spray with the injection pressure up to 120 MPa under high pressures and high temperatures relevant to CI engines in a constant volume vessel. The spray model was tuned and validated against the observation results as well as experimental data we have reported previously, such as spray penetration, liquid length, ignition delay and combustion process. We also developed a reduced kinetic reaction scheme of DME oxidation, based on the latest detailed kinetic mechanism by Burke et al [24]. Finally, DME spray combustion simulation in a constant volume vessel and in a CI engine was conducted using the spray model coupled with the reduced reaction scheme.

FUEL PROPERTY OF DME

DME is the simplest ether with the chemical formula CH_3OCH_3 . DME is a gas at normal temperatures and pressures. To use for CI engines, it must be handled as a liquid under pressures above 0.5 MPa. Fuel properties of liquefied DME are different from those of diesel fuel, as shown in Table 1. DME has lower density and lower heating value than diesel fuel. In order to obtain the same output, 1.8 times the injection quantity of diesel fuel is required. DME is highly compressible and its bulk modulus is low. Therefore, it is hard to increase the injection pressure. The maximum injection pressure of current DME engines is at about 60 MPa [9], much lower than that of diesel fuel engines. A nozzle diameter of the fuel injectors must be increased to compensate for the deficiency in energy content. It is thought to be disadvantaged in terms of air entrainment in the spray.

DME is highly volatile because the surface tension is lower and the vapor pressure is much higher than those of diesel fuel. There is a potentially strong effect on breakup and evaporation process.

Table 1. Properties of DME and diesel fuel [17]

Fuel	DME	Diesel Fuel
Chemical formula	CH_3OCH_3	-
Cetane number	60.6	55
Stoichiometry A/F ratio	9	14.6
Liquid density [g/cm ³ @293 K]	0.67	0.8-0.84
Lower heating value [MJ/kg]	28.9	42.7
Kinetic viscosity [cSt]	0.25	3
Bulk modulus [10^8N/m^2]	6.37	14.9
Vapor pressure [kPa]	530	0.13
Surface tension [mN/m]	10	28.2

OBSERVATION OF DME SPRAY

The authors have investigated the DME spray combustion under pressures and temperatures relevant to actual engines in a constant volume vessel to understand the spray development and combustion characteristics [18][19][20]. Microscopic ultra-high speed observation was also made to identify differences in breakup behavior between DME and diesel fuel spray. In the present study, we conducted high speed observation of high-injection-pressured DME spray up to 120 MPa.

In this paper, we summarized the past observation made by the authors. These were utilized to evaluate the spray combustion model developed in this study, in conjunction with the newly obtained observation of high-pressure-injection spray.

Experimental Setup and Optical Method

Schematic diagram of the experimental apparatus is shown in Figure 1. High-temperature and high-pressure ambient conditions were made inside the constant volume vessels. The fuel was injected into the vessels from the injector mounted at the center on top of the vessel, using a common rail DME injection system developed by DENSO Co., Ltd.

The spray was imaged with a high-speed video camera through the synthetic quartz window on the side. Two optical methods were employed; diffused-light shadowgraph method and parallel-light shadowgraph method. The diffused-light shadowgraph method was applied to image the droplets in the spray. With this method, well diffused light is provided from behind the spray. The droplets blocks the light and yields shadows, while schlieren effect is eliminated because back light is well diffused. The parallel-light shadowgraph method, ordinary shadow graph technique, was applied to image the gas-phase spray, as well as fuel droplets, to capture the shape of the spray and penetration length.



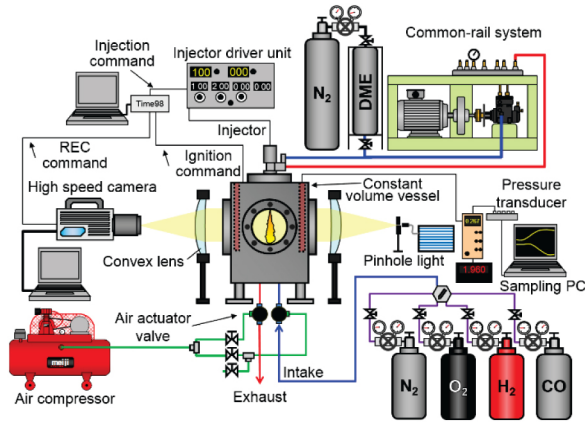


Figure 1. Experimental setup for spray observation

The constant volume vessels used in this study are shown in Figure 2. Two constant volume vessels were employed. The smaller one is intended for microscopic observation, and the larger one is intended for macroscopic observations.

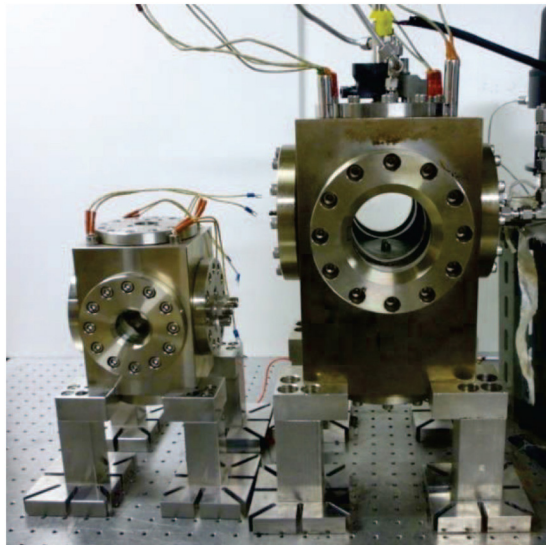


Figure 2. Constant volume vessels used for spray observation

The smaller vessel has 24 mm-thick quartz windows with a view field of 39 mm diameter. A high-power microscope lens with short focal length can be applied because the quartz window is thin. Nitrogen inside the vessel is heated up to 500 K and 5 MPa with four 2 kW electric heaters equipped at four corners of the vessel. Breakup and evaporation behavior near the injector orifice was microscopically observed with this system.

The larger constant volume vessel with a view field of 80 mm diameter was used for macroscopic observations of the spray development and combustion. The pressures and temperatures inside the vessel can be raised up to 10 MPa and 1000 K, by pre-combustion of H_2 , O_2 , CO , N_2 mixture. The oxygen concentration after pre-combustion was varied by the mixture composition.

Microscopic Observation [18]

Experimental Conditions

Ultra-high-speed microscopic observations were conducted to understand the break-up process of DME spray. The experimental conditions of microscopic observation are shown in Table 2. The experiments were conducted at nitrogen ambient under the pressure-temperature condition of 4.32 MPa-444 K. The ambient density was 34.159 kg/m^3 , equal to a density at 8.8 MPa-920 K of a typical supercharged diesel engine condition [19].

For imaging the breakup behavior, a nano flash light with exposure duration of 18 ns was employed for a light source. The spray movie was taken at a frame rate of 4000 fps synchronized with the flash light, with resolution of 800×600 pixels and a view field of $3.53 \times 4.49 \text{ mm}$. For imaging the development process at the early stage of the spray near the injector orifice, the movie was taken at a frame rate of 1,000,000 fps, with resolution of 360×410 pixels and a view field of $4.49 \times 3.87 \text{ mm}$, using a continuous light source.

A single-hole injector with the orifice of 0.35 mm diameter was used for DME injection. The injection pressure was set at 60 MPa, which was determined by reference to the latest DME engine [9].

Table 2. Experimental conditions of spray observation

Fuel	DME	
	Diesel fuel	
Ambient pressure [MPa]	4.32	
Ambient temperature [K]	444	
Exposure time [ns]	18	100
Frame rate [kfps]	4	1000
Number of pixel [pixel]	800X600	360X410
Nozzle diameter [mm]	0.35	
Injection pressure [MPa]	60	

The Microscopic Observation Results

DME spray images near the injector orifice with a high-speed frame rate of 1,000,000 fps are shown in Figure 3. Just after the start of injection, the spray spouted from the orifice is pressed against ambient gas and expands laterally. Then, the spray tip accelerates due to the overtaking of spray of following injection. At the same time, minuscule droplets are formed by the breakup of the spray core. Diesel fuel spray at the same injection condition of Figure 3 is shown in Figure 4. The breakup actively occurs and more droplets are formed compared with DME spray.

Figure 5 shows DME spray images with exposure duration of 18 ns at the position of 18.7-22.3 mm from the injector orifice, near the inflection point of spray penetration curve where the interference between fuel spray and ambient gas actively occurs, at 1.5 ms and 2.5 ms after the start of injection. Wavy disturbance occurs and DME evaporates on the outer edge of the spray. No droplets are observed.

Fuel : **DME** / Frame rate : **1,000,000 fps**
 Ambient condition : **4.32 MPa - 444 K**
 Orifice diameter : **0.35 mm** / Injection pressure : **60 MPa**

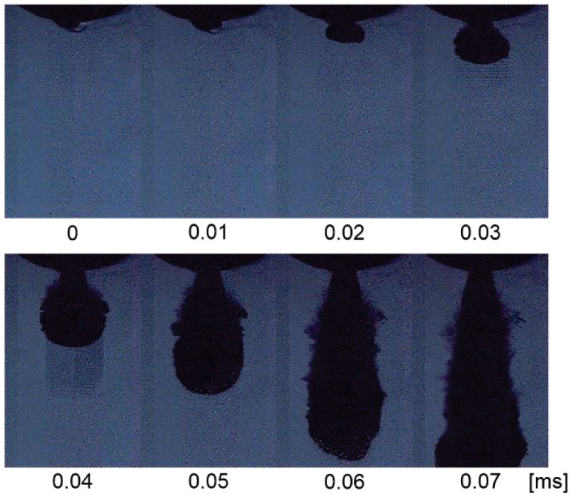


Figure 3. DME spray at the initial stage of injection [18]

Fuel : **Diesel** / Frame rate : **1,000,000 fps**
 Ambient condition : **4.32 MPa - 444 K**
 Orifice diameter : **0.35 mm** / Injection pressure : **60 MPa**

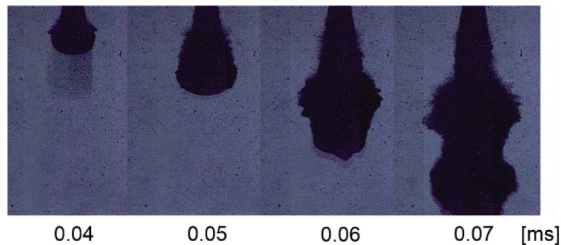


Figure 4. Diesel spray at the initial stage of injection [18]

It is well known that liquid spray formation starts from breakup of liquid core into droplets and then the droplets breakup into smaller ones, so called the secondary breakup. The fuel evaporates as the droplet size decreases, because the surface area of the droplets increases. The spray formation process of DME, on the other hand, appears to be unlike the case of ordinary liquid fuel. DME evaporates without the secondary breakup process. DME has low surface tension and the Weber number is high. The droplet size is thought to be smaller. The vapor pressure is much higher than of diesel fuel. Therefore, the evaporation speed is considered to be faster than the breakup speed.

Frame rate : **4000 fps** / Ambient condition : **4.32 MPa - 444 K**
 Orifice diameter : **0.35 mm** / Injection pressure : **60 MPa**
 Observation position : **18.7-22.3 mm under the nozzle**

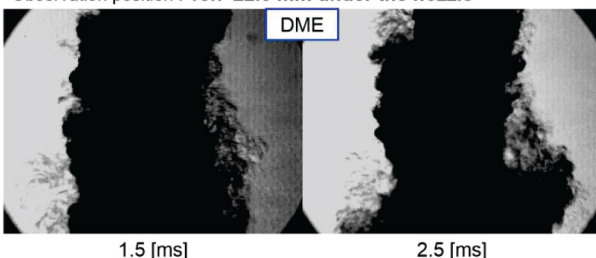


Figure 5. DME spray image with high exposure time of 18 ns around breakup length [18]

Macroscopic Observation

The Observation of DME and Diesel Spray [20]

Microscopic observation of DME spray was conducted in order to understand the development process and combustion process under 6.0 MPa-920 K. A single-hole injector with an orifice diameter of 0.35 mm was used and injection pressure was 60 MPa. Diesel spray observation was also conducted for comparison using a single-hole injector with an orifice diameter of 0.173 mm, and the injection pressure of 200 MPa. The injection conditions are typical of DME and diesel engines. DME is made to be injected with bigger orifice and lower injection pressure. The injection energy is almost the same for both cases.

Non-combustion sprays of DME and diesel fuel are shown in Figure 6 and 7, respectively. There is no significant difference in spray shape. The spray tip penetration lengths and liquid length measured from the figures are shown in Figure 8. Liquid length of DME spray is about 20 mm, shorter than that of diesel spray. As mentioned before, it is obvious that DME evaporates faster than does diesel fuel. Penetration length of DME is slightly shorter than that of diesel fuel. This is because DME spray has a slightly wider spray angle and its momentum is small due to the small liquid density.

Diesel and DME spray combustion observations are shown in Figure 9. Ignition delay times are almost the same for both fuel types. There is a distinct difference in flame luminosity. Diesel fuel spray has highly luminous flame, whereas DME has non-luminous flame. This exemplifies that DME combustion forms no soot.

Fuel : **DME / Non-combustion**
 Ambient condition : **6.0 MPa-920 K**
 Inj. pressure : **60 MPa** / Orifice diameter : **0.35 mm**

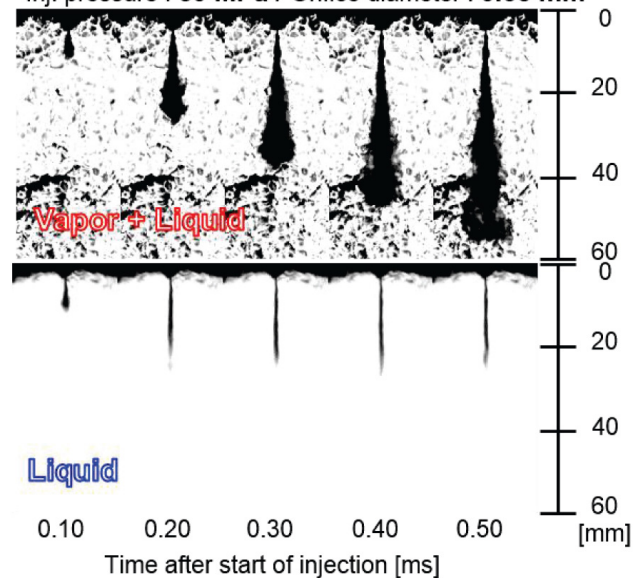


Figure 6. Non-combustion DME spray [20]