



## Explosion and detonation characteristics of dimethyl ether

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### ARTICLE INFO

#### Article history:

Received 6 March 2008

Received in revised form 25 July 2008

Accepted 30 July 2008

Available online 6 August 2008

#### Keywords:

Dimethyl ether

Propane

Detonation

Explosion

$K_G$  value

### ABSTRACT

In this study, the explosion and detonation characteristics of dimethyl ether (DME) were experimentally investigated. A spherical pressure vessel with an internal volume of 180 L was used as the explosion vessel. Therefore, tubes 10 m in length with internal diameters of 25 mm and 50 mm were used as detonation tubes. In addition, we compared the characteristics of DME with those of propane since DME is considered as a substitute fuel for liquid petroleum gas (LPG). At room temperature and atmospheric pressure, the maximum explosive pressure increased tenfold. The explosion index ( $K_G$  values), an indicator of the intensity of an explosion, was larger than that of propane, indicating that the explosion was intense. No experimental study has been conducted on the detonation behavior of DME so far, but this research confirmed a transition to detonation. The detonation characteristics were similar to the characteristics of the Chapman–Jouguet detonation, and the concentration range for detonation was from 5.5% to 9.0%.

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### 1. Introduction

Recently, a variety of studies have been conducted on converting pyrolysis gas and biomass into gaseous fuels such as hydrogen, methane, and dimethyl ether (DME) or liquid fuels such as methanol, ethanol, and biodiesel, which are sources of energy that are less polluting and more environmentally friendly; the main component of pyrolysis gas is carbon monoxide and pyrolysis gas is obtained from natural gas. Of these fuels, DME can be easily produced from a primary fuel such as natural gas. DME resembles liquid petroleum gas (LPG) – a mixture of propane and butane – with regard to its boiling point and vapor pressure characteristics, which makes it easy to handle. It also shows promise as a diesel alternative since it has a low self-ignition temperature and does not generate particulate matter (PM).

However, since DME has been primarily used as an aerosol propellant, it has almost no history as a fuel. Therefore, we must proceed to elucidate the properties and safety features of DME because if it is to be utilized on a large scale, adequate measures must be developed for its safe use. A number of studies have been conducted on the properties and combustion characteristics of DME, but a very small number of studies involve experimental investigations into its explosive and detonation characteristics. In particular, investigations have not confirmed whether DME can detonate; therefore, fundamental data must be obtained on the

conditions under which DME will detonate in practical applications. Few investigations have been reported on the detonation properties of DME. Studies have been conducted on DME–oxygen mixtures [1,2]. However, the number of studies on DME–air mixtures is few.

In this research, explosion phenomena in a DME–air mixture were investigated and the explosion index ( $K_G$  value) was obtained by measuring the explosion pressure and the rate of explosion pressure rise. We also investigated whether DME could actually detonate in a detonation test tube. In addition, we compared the characteristics of DME with those of propane since DME is considered as a substitute fuel for LPG.

### 2. Experimental setup

#### 2.1. Explosion test

Fig. 1 shows a schematic of the apparatus for the explosion tests, which employs a spherical vessel. The spherical pressure-resistant explosion vessel had an internal diameter of 700 mm and an internal volume of 180 L and had ignition electrodes at its center. For spark discharge ignition, two stainless discharge electrodes, both with a pointed tip, were positioned with a 7 mm gap between them, and a direct current was discharged with a maximum voltage of 20 kV at 1 mA for an interval of 0.1–0.5 s. For nichrome fuse wire ignition, a nichrome wire with a diameter of 0.4 mm and length of approximately 60 mm was connected across the electrodes, and a voltage of 12 V (DC) was applied across it. A strain gauge pressure transducer (Kyowa Electronic Instruments, PE-30KF) was

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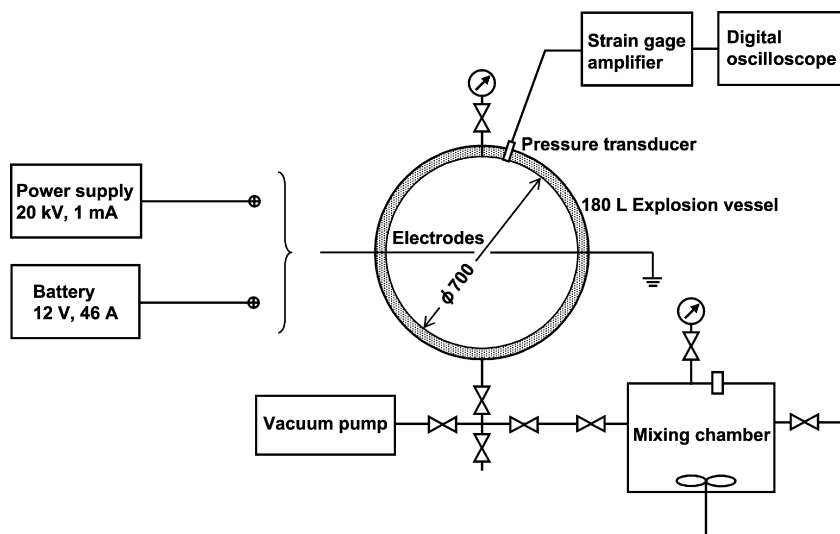


Fig. 1. Schematic of experimental apparatus for explosion test.

used for measuring the pressure, and the amplified output was recorded on a digital oscilloscope (Yokogawa Electric Corporation, DL708).

## 2.2. Detonation test

Fig. 2 shows a schematic of the apparatus used for the detonation tests; the apparatus employs detonation tubes. The detonation tube A has 50 mm in diameter and 10,000 mm in length. On the other hand, the detonation tube B has 25 mm in diameter and 5000 mm in length. The combustible mixture was ignited by a nichrome fuse

wire at the end of the tube. The pressure was measured by piezoelectric pressure sensors (PCB Piezotronics, 111A24) mounted along the wall of the tube. The pressure waveform obtained from the pressure sensors was amplified and recorded on a digital oscilloscope.

In experiments that employed either the spherical vessel or the tube, air was first evacuated, and subsequently, gas that had been premixed to the prescribed concentration in a mixing container was introduced. When the atmospheric pressure was reached, the valve was closed and the mixture was ignited. The composition of the gas mixture was determined by the partial pressure method. The experiments were conducted at room temperature.

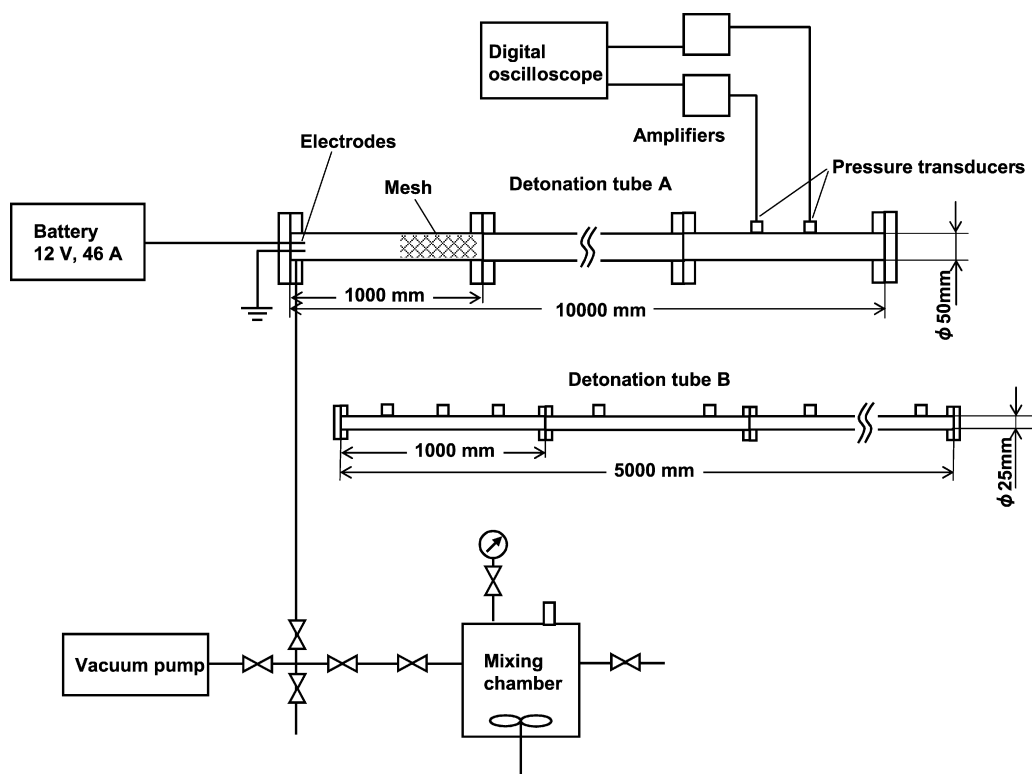


Fig. 2. Schematic of experimental apparatus for detonation test.

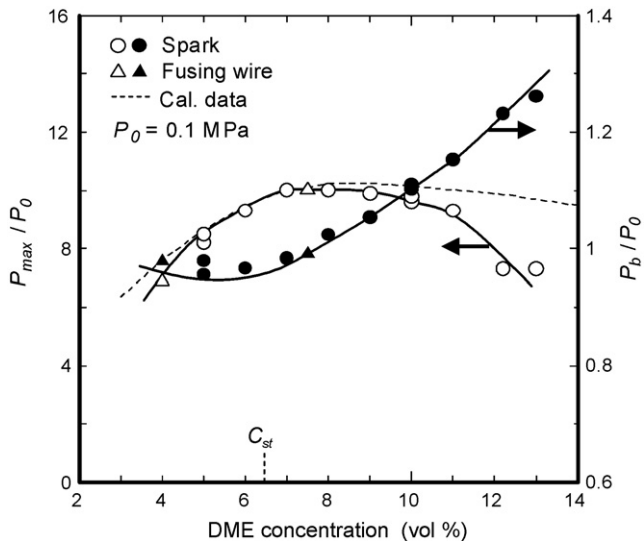


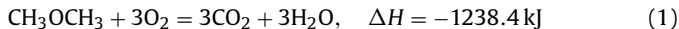
Fig. 3. The dependence of maximum pressure ratio and ultimate pressure ratio on DME concentration.

### 3. Results and discussion

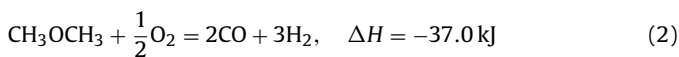
#### 3.1. Explosion characteristics

Fig. 3 shows the variations in the maximum explosion pressure  $P_{max}$  and the ratio of the ultimate pressure  $P_b$  to the initial pressure  $P_0$  with the DME concentration (all pressures referred to hereinafter are absolute pressures). The dotted line in the graph shows the explosive pressure calculated using the NASA Chemical Equilibrium with Applications (CEA) code [3]. Although the stoichiometric concentration of air is 6.54 vol.%, the explosion pressure reaches its maximum value at a higher concentration of approximately 7.5%. From the lower explosion limit to approximately the stoichiometric composition, the experimental results and calculated values are comparatively consistent. The large discrepancy that arises towards the upper limit suggests that the reaction at higher concentrations is not taking place according to the chemical equilibrium. The main cause for this can be presumed to be that the combustion is incomplete and the combustion speed is low. Note that very little difference is observed between the two ignition methods employed.

The DME combustion reaction can be given as follows:



According to reaction (1), the post-explosion pressure should fall due to the production of water, but in practice, it rose with the concentration, as can be observed in Fig. 3. The product was not analyzed. However, judging from the equilibrium composition determined by chemical equilibrium calculations, as shown in Fig. 4, and considering that the production of  $\text{H}_2$  increases with the concentration and that the post-explosion pressure rises, the following reaction can be presumed to have contributed to the increases:



A small amount of heat is generated according to reaction (2); the heat can be considered to be linked to the flame propagation toward the upper limit.

Fig. 5 shows the results of the calculation of the explosion index and the maximum rate of the explosion pressure rise  $[(dP/dt)_{max}]$ . This figure also contains the burning velocities for DME published

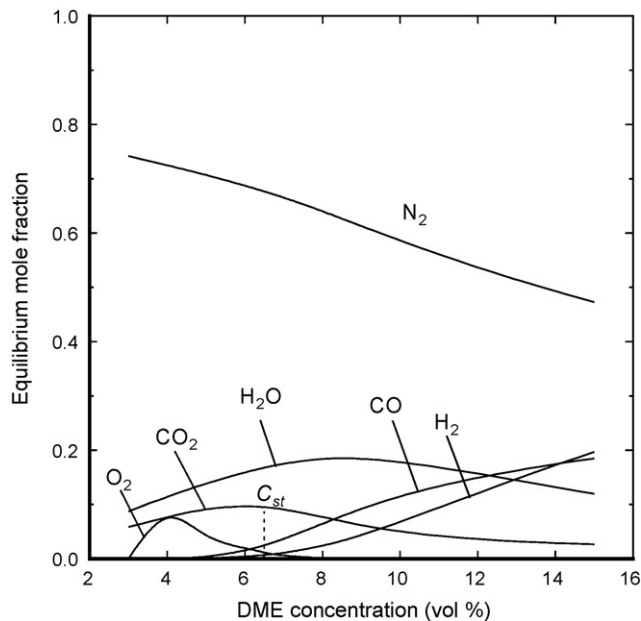


Fig. 4. The dependence of equilibrium mole fractions on DME concentration.

available values [4] for comparison.  $(dP/dt)_{max}$  was found from the maximum gradient of the rising curve of the explosion pressure waveform, and  $K_G$  was found using the following formula:

$$K_G = \left( \frac{dP}{dt} \right)_{max} \times V^{1/3}$$

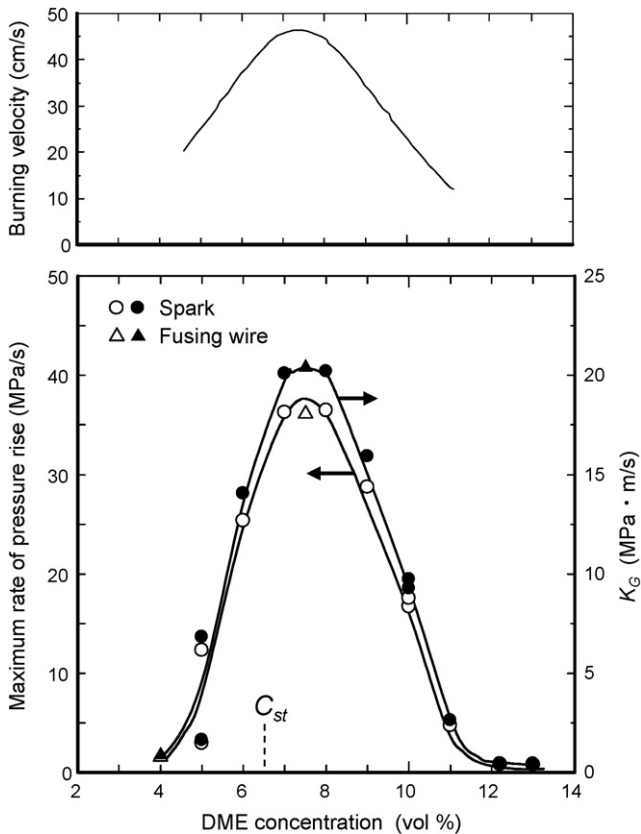


Fig. 5. The dependence of rate of pressure increase,  $K_G$  value, and burning velocities on DME concentration.

**Table 1**  
 $K_G$  value comparison between DME and propane

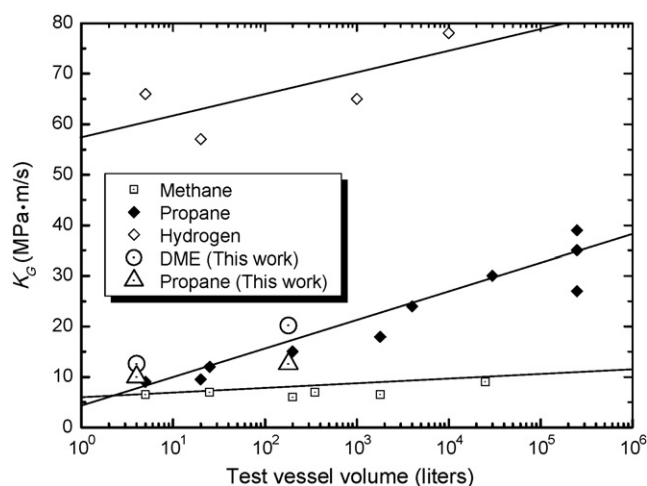
Gas	Volume, shape	Maximum pressure value, $P_{max}$ (MPa)	$K_G$ (MPa m/s)	Note
DME	180 L, spherical	10.0	20.2	This work
	22 L, barrel	8.9	10.8	Ref. [4]
	4 L, spherical	9.4	12.6	Our other work
Propane	180 L, spherical	9.6	15.1	This work
	22 L, barrel	8.2	7.6	Ref. [4]
	4 L, spherical	8.9	10.0	Our other work

where  $V$  is the internal volume of the vessel. The maximum rate of the explosion pressure rise also occurred on the higher concentration side relative to the stoichiometric composition, reaching 37 MPa/s. No difference was observed between the different ignition methods. The  $K_G$  value of DME (stoichiometric) that Senecal et al. [5] reported was 10.8 MPa m/s, but a considerably higher value was obtained from the measurements of this experiment. However, the  $(dP/dt)_{max}$  value reported by Senecal et al. was 38.5 MPa/s and this was almost the same as the value obtained in this work. In other words, although the  $K_G$  values were used because the obtained values were stable regardless of the internal volume of the measurement vessel [6], in practice, the dimensions of the vessel could be considered to influence the values.

Table 1 shows a comparison between the maximum explosion pressures and the  $K_G$  values for DME and propane. For propane, a  $K_G$  value of 7.6 MPa m/s was reported [5], but the value obtained by the method used here was 15.1 MPa m/s. In the data of a 4-L spherical vessel, we used other vessel and obtained the  $K_G$  value. Fig. 6 shows a comparison of the results obtained in the present study with those of another study [7]. Variations can be observed in the  $K_G$  value depending on the volume of the vessel, similar to the case of DME.

### 3.2. Detonation characteristics

An example of the pressure profiles obtained for the DME–air mixtures when the detonation tube A and the stoichiometric composition were used is shown in Fig. 7. The pressure sensors were positioned 9400 and 9600 mm from the ignition end of the tube. The time elapsed after the ignition is indicated on the horizontal axis. The pressure wave generated by the flame acceleration was reflected off the ends of the tube; this caused the tube to vibrate and gradually raised the pressure because both ends of the tube



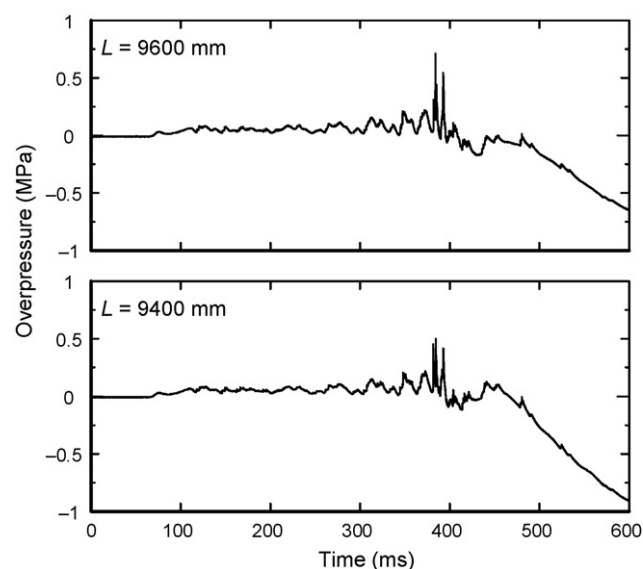
**Fig. 6.** Effect of test volume on measured  $K_G$  value.

were closed. The pressure profiles do not show a sharp rise, and the detonation transition is not confirmed.

Similar experiments were also conducted using propane–air gas mixtures, but no deflagration-to-detonation transition was observed in the 10-m tube. As for propane, no transition to detonation occurred when a tube having the same diameter (50 mm) as the one used here but with a length of 18 m was used [8].

A square wire mesh (4 mesh/in., the wire diameter was 1 mm) rolled cylindrical (the roll length was 300 mm), as the Shchelkin spirals is positioned in the tube 1000 mm from the ignition end to accelerate the flame propagation. The pressure profiles obtained in this experiment are shown in Fig. 8. A spike-like pressure change can be observed, confirming the transition to detonation. In other words, the pressure reaches a maximum from the shockwave of the detonation wave front, and then falls off to a stable level around the Chapman–Jouguet pressure,  $P_{CJ}$ . The second peak can be attributed to reflected waves from the end of the tube.

Fig. 9 shows the detonation pressure and detonation velocity when the DME concentration is varied. The dotted line in the diagram indicates the theoretical detonation pressure, which is calculated by using the NASA CEA code [3]. The conditions for the deflagration-to-detonation transition depend on the shape and dimensions of the tube [9], but the range for detonation in the conditions used in these experiments is between around 5.5% and 9.0%. In the case of the deflagration-to-detonation transition, the pressure and wave velocity roughly match the theoretical values, and the maximum pressure occurs at a higher concentration than the stoichiometric composition, similar to the case of explosive pressure.



**Fig. 7.** Pressure profiles of DME–air deflagration.

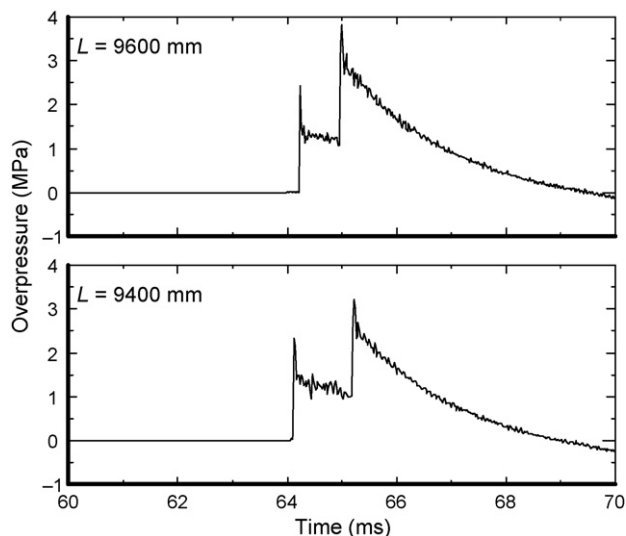


Fig. 8. Pressure profiles of DME-air detonation.

In order to examine the characteristics of the detonation transition and compare them with those of DME and propane, the experiments were conducted using stoichiometric fuel/O<sub>2</sub> mixtures or fuel/O<sub>2</sub>/N<sub>2</sub> (50% or 75% N<sub>2</sub> in the total mixture) mixtures. In this experiment, detonation tubes with a diameter of 25 mm were used and the wire mesh was not installed. In the case of fuel/O<sub>2</sub> mixtures and fuel/O<sub>2</sub> mixtures with 50% N<sub>2</sub> in the total mixture, the detonation transition was confirmed in both DME and propane. Figs. 10 and 11 show the velocity profile of the combustion wave as it traveled down the tube. Each data point corresponds to the average velocity between adjacent pressure sensors. The dashed and dotted line indicates the Chapman–Jouguet velocity for each mixture. The DDT run-up distance is within 250 mm for fuel/O<sub>2</sub> mixtures. In the case of DME–O<sub>2</sub>–50% N<sub>2</sub>, the DDT run-up distance ranges from 0.625 m to 1 m. On the other hand, in the case of propane–O<sub>2</sub>–50% N<sub>2</sub>, it ranges from 1 m to 1.5 m. As a result, it appears that the DDT run-up distance of DME is smaller than that of propane but the detonation velocity of DME is smaller than that of propane.

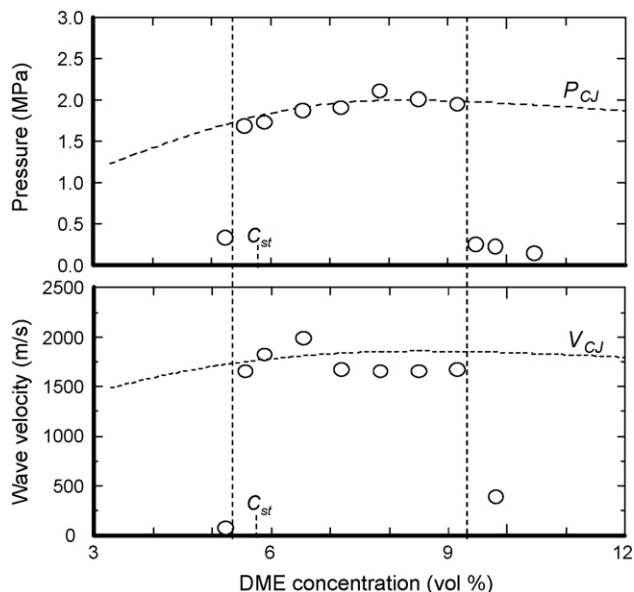


Fig. 9. Dependence of peak overpressure and velocity on DME concentration.

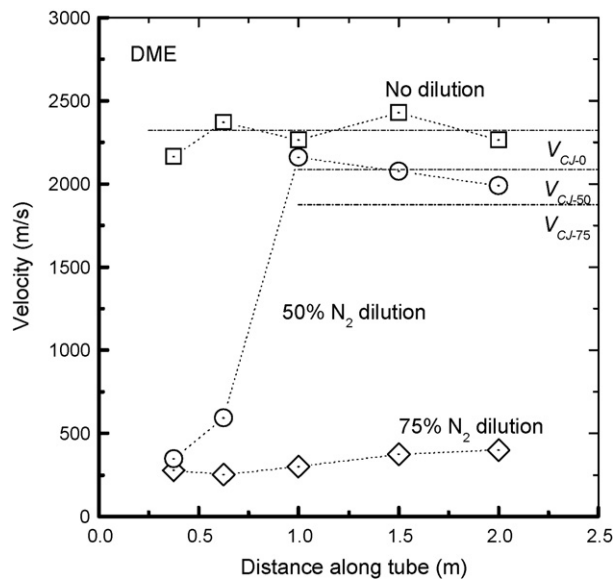


Fig. 10. Velocity profiles for DME–O<sub>2</sub> and DME–O<sub>2</sub>–N<sub>2</sub>.

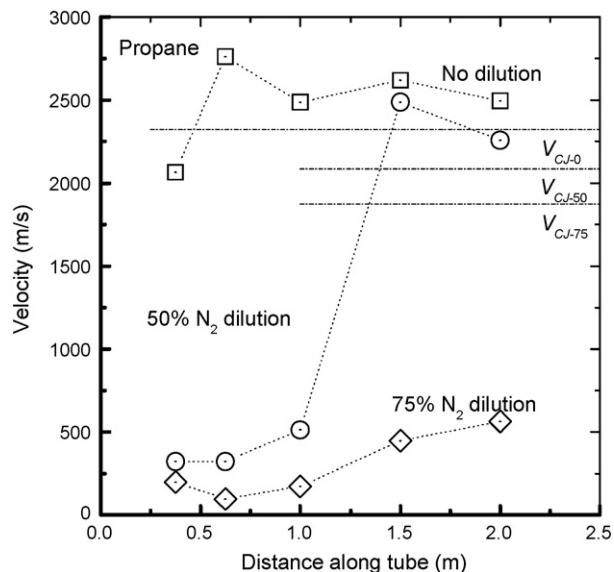


Fig. 11. Velocity profiles for propane–O<sub>2</sub> and propane–O<sub>2</sub>–N<sub>2</sub>.

#### 4. Conclusions

A study was conducted on the explosion and detonation of DME in air. At room temperature and atmospheric pressure, the maximum explosive pressure increased tenfold. The  $K_G$  values, an indicator of the intensity of an explosion, were larger for DME as compared to those of propane, indicating that the explosion was intense. No experimental study has been conducted on the detonation behavior of DME so far, but this research confirmed the transition to detonation by using obstacles. The detonation characteristics were similar to the CJ characteristics, and the concentration range for detonation was from 5.5% to 9.0%. In addition, the run-up distance of DME was smaller than that of propane.

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