An experimental investigation of the explosion characteristics of dimethyl ether-air mixtures

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Abstract

In this work, experiments are performed to study the explosion characteristics of dimethyl ether (DME)-air mixtures using a standard 20-L spherical explosion test apparatus. The experimental data reported in this paper includes: the maximum explosion pressure ($p_{\text{max}}$), flammability limits, maximum rate of pressure rise ($\frac{dp}{dt}_{\text{max}}$), and combustion properties (i.e., laminar burning velocity, flame radius) of DME-air mixtures at different initial conditions. The experimental results indicate that the variation between $p_{\text{max}}$ and DME concentration ($C_{\text{DME}}$) exhibits a typical inverse “U” shaped behavior, with the peak $p_{\text{max}}$ at slightly larger than the stoichiometric concentration. $p_{\text{max}}$ is also found to decrease as the initial pressure goes down. As the initial pressure decreases from 100 kPa to 40 kPa, the lower flammability limit (LFL) is observed to vary slightly, while the upper flammability limit (UFL) is found to have a more significant drop. The relation between ($\frac{dp}{dt}_{\text{max}}$) and $C_{\text{DME}}$ behaves similarly as that of $p_{\text{max}}$ as a function of $C_{\text{DME}}$, and the explosion pressure rises more abruptly at higher initial pressure. A satisfactory agreement is also found between the laminar burning velocity determined experimentally from the pressure measurement and that computed by PREMIX simulations. The present experimental results also show that the increase of the dimensionless radius of the flame is slower at higher initial pressure.

Keywords: Dimethyl ether; Maximum explosion pressure; Flammability limits; Maximum rate of pressure rise; Laminar burning velocity; Flame radius.
1 Introduction

Dimethyl ether (DME: CH₃OCH₃) is a promising oxygenated fuel that has the potential to be used as an alternative to natural gas for power production and as a substitute for diesel fuel. DME has high oxygen content of 35% by weight, making the combustion smokeless and a high tolerance to exhaust gas recirculation [1]. The use of DME has been proven to significantly decrease particulate formation, nitrogen or sulfur oxides (NOₓ and SOₓ), and carbon monoxide (CO) emission [2, 3]. DME also has a high Cetane number of 55 to 60 and a boiling point of -25 °C. These properties are ideal for fast mixture formation, reduction in ignition delay, and cold start for diesel engines [4].

Due to its potential as a future alternative fuel, the combustion characteristics of DME have attracted significant attention in recent years [5-10]. A number of experimental and numerical studies can be found in the literature on the combustion and emission characteristics of DME under engine conditions [11-13]. Fundamental properties such as flammability and laminar burning velocities [14-17], and combustion processes of DME under turbulent conditions [3] were also reported. Detailed chemical mechanisms for low and high temperature DME oxidation have been developed and validated [18, 19], and a recent mechanism for DME mixture at high pressures was also constructed by Burke et al. [20]. Furthermore, the effects of DME addition on the high-temperature ignition and burning properties of methane-air mixtures were studied experimentally and numerically [21]. Premixed and non-premixed ignition of methane/DME binary fuel blends with hot air has been investigated through numerical simulation with detailed chemistry and complete thermo-chemical as well as transport properties [22]. Detonation velocities and characteristic cell sizes of DME-oxygen and DME-air mixtures have been measured by Ng et al. [23] and Diakow et al. [24], and the explosion and detonation
characteristics of DME were experimentally investigated using a 180-L spherical vessel and a large-scale detonation tube by Mogi and Horiguchi [25]. In addition, experiments were also carried out to examine the leakage and explosion of liquid DME [26].

While DME flames have been studied extensively, comparatively little information exists on the explosion characteristics, e.g., flammability limits, maximum explosion pressure, $p_{\text{max}}$, maximum rate of pressure rise, $(dp/dt)_{\text{max}}$ of DME at various initial conditions. The knowledge of the explosion characteristics of DME is of importance to ensure the safety in industries that produce or use it. A realistic assessment of the explosion hazards of DME is necessary for preventive measures of explosion accidents and the design of effective mitigation schemes. Among those aforementioned combustion and explosion characteristics, a key combustion property is the laminar burning velocity ($S_L$) which is the velocity of a steady one-dimensional adiabatic free flame propagating in the doubly infinite domain [27]. It received particular attention not only because it represents a basic characteristic property (e.g., reactivity, diffusivity, and exothermicity) of the premixed combustible gasses [28], its accurate knowledge is also essential for engine design, modeling of turbulent combustion, and validation of chemical kinetic mechanisms. In addition, the determination of laminar burning velocity is very important for the analysis and calculations used in the field of explosion protection [29]. Besides experimental measurement, the laminar burning velocity can also be estimated by numerical calculation through PREMIX simulations [30], or by semi-empirical mathematical model [31, 32]. The results obtained from experimental measurement and numerical calculation can then be compared for validation and assessment, together with data reported in the literature [4, 33].

The objective of the present study was twofold. First, the explosion parameters of DME-air mixtures are systematically measured from experiment. The explosion parameters include: the
maximum explosion pressure $p_{\text{max}}$, both lower flammability limit (LFL) and upper flammability limit (UFL), and the maximum rate of pressure rise $(dp/dt)_{\text{max}}$. Second, the combustion characteristics (i.e., laminar burning velocity and the evolution of flame radius) are examined in detail under different initial conditions. The laminar burning velocity obtained from different methods are also compared and discussed.

2 Experimental details

2.1 Experimental setup

Measurements of the explosion parameters in DME-air mixtures were carried out in a standard 20-L explosion spherical vessel conforming to the international standard ISO6184-1, see Fig. 1. It essentially consists of an explosion chamber, an electric ignition system, a control unit, a data acquisition system, a release valve, a vacuum pump and an air compressor. High-voltage electric spark was used to supply ignition energy as in previous studies [34-39]. The igniter was mounted at the center of the spherical bomb and a spark energy of 10 J, estimated from $1/2 \, CU^2$ (“$C$” and “$U$” refer the capacitance and voltage, respectively. $C = 0.1102 \times 10^{-3}$ F, $U = 426$ V), was delivered by an electric ignition system.

2.2 Experimental procedure and conditions

For the explosion experiments, gas concentrations were regulated by the gas partial pressures. The purity of the DME used in this experiment is 99.8 %. During the experiments, the explosion pressure evolutions were measured by a PCB pressure transducer installed in the vessel wall and recorded by a data acquisition system for each shot. These data yielded values of the maximum explosion pressure and maximum rate of pressure rise as illustrated in Fig. 2. This figure shows
a typical pressure history of the DME-air of $C_{\text{DME}} = 10\%$ at an initial pressure $p_0$ of 100 kPa. The combustion time $t_c$ is defined as the period from ignition to the time when the overpressure reaches its maximum. The measurements were repeated at least 3 times, and results were presented in the figures with error bars determined by the standard deviation. The main sources of the small variation can stem from the effect of wall cooling, ignition source, the degree of mixture homogeneity and asymmetry [40]. In this study, a wide range of initial conditions of DME-air mixtures were used. The initial pressure ranges from 40 kPa to 100 kPa, and fuel concentrations are from 3 to 19.5 %.

3 Results and discussion

3.1 Maximum explosion pressure

Gas explosion max-overpressure is an important parameter of evaluating the explosion hazard. It reflects the energy distribution of explosive waves in their propagation process [41-46]. The measurement of the explosion pressure in quiescent DME-air mixtures with various compositions at the ambient condition are summarized in Table 1. In this table, $p_{\text{max}}$ and its corresponding $t_c$ are directly obtained from the pressure history. For comparison, the adiabatic pressure $p_{\text{ad}}$ is also given and is calculated from thermo-chemical analysis using the GASEQ software [47]. These experimental data of $p_{\text{max}}$ are also compared with those reported by Mogi and Horiguchi [25], and a curve fit of $p_{\text{max}}$ using smoothing splines is also given for better comparison, see Fig. 3. The explosion pressure reaches its maximum value at a composition of 7.5 %, which is slightly larger than the stoichiometric concentration (6.5 %). A similar behavior is also observed by Mogi and Horiguchi [25] in their 180-L spherical vessel. Near the stoichiometric condition, both the present data as well as the results by Mogi and Horiguchi [25] agree well with the adiabatic explosion pressure determined from chemical equilibrium within.
the experimental uncertainties. The experimental measurement starts to deviate from the
adiabatic pressure at off-stoichiometric conditions, prominently on the rich side. As pointed out
by Mogi and Horiguchi [25], at those conditions the combustion speed decreases and the event
departs from its constant-volume explosion character. Incomplete combustion and the effect of
cooling also give rise to this discrepancy, which are susceptible to the scale of the apparatus. In
fact, it can also be seen from Fig. 3 that, the results of $p_{\text{max}}$ from this study are slightly larger
than those of Mogi and Horiguchi near stoichiometric concentration, though within
experimental uncertainties. A contrary behavior is also observed as the composition tends to
both the fuel lean and rich sides. It is noteworthy that in [25], Mogi and Horiguchi used a 180-L
spherical vessel, while the present study is performed using a 20-L one. Thus, the discrepancy at
off-stoichiometric conditions can be caused by the wall cooling effects. Near stoichiometric
conditions, the combustion speed is high and the cooling rate has less influence on the
overpressure. However, for incomplete combustion where the temperature is lower (i.e., at off
stoichiometric conditions), the combustion speed becomes slower, which allows a longer time
scale of the phenomenon for the cooling effect to come into play. The faster cooling of a smaller
volume in the 20-L chamber, as compared to the 180-L large-scale apparatus used by Mogi and
Horiguchi [25], thus results in a lower overpressure.

Figures 4 to 6 show the results of $p_{\text{max}}$ for different DME compositions at an initial pressure
lower than the atmospheric condition, i.e., 80 kPa, 60 kPa and 40 kPa. To show the general trend
in the experimental data, curve fits using a third order polynomial are also plotted for better
visualization. Note that there is no previous experimental data at those pressure values for direct
comparison. Therefore, the measured data are merely compared with the chemical equilibrium
results obtained using the GASEQ software [47]. Similarly, large difference is observed as the
condition moves toward the LFL and UFL. Again, the theoretical maximum explosion pressure
determined from the equilibrium calculation is based on the hypothesis of ideal adiabatic
explosion. As the composition tends to fuel-lean or fuel-rich sides, not only incomplete reaction
occurs but also the heat loss to the surrounding can affect the explosion process, making the
measured values different from the chemical equilibrium calculation of an ideal adiabatic
explosion. It is observed from Figs. 4 to 6 that the value of $p_{\text{max}}$ goes down as the initial pressure
decreases. This observation perhaps suggests that the faster reactivity induced by the higher
initial pressure reduces the effect of heat losses on the explosion process. Hence, the higher
initial pressure may maintain higher explosion temperature, which in turn results in the rise of
overpressure.

3.2 Flammability limits

Table 2 shows the LFL and UFL for the DME-air mixture at different initial pressures. These
limits were determined when half of the shots at the same condition indicate no occurrence of
explosion. It is observed that the LFL has only a small fluctuation as the initial pressure
decreases, i.e., only a small increase from 3.5 % to 3.75 % as the initial pressure changes from
100 kPa to 40 kPa. However, the UFL is found to have relatively a more significant drop, which
changes from 19 % to 12.5 %. Reducing the initial pressure is found to narrow the interval width
of these two limits. It is worth to point out that this observed behavior is similar to hydrogen/air
[48] in which the lower flammability limit is not significantly sensitive to the initial pressure,
while the latter has more significant effect on the UFL. From the chemical kinetic point-of-view,
the effect of pressure increase has an influence on the reaction rates, especially those involved
third body collisions. As shown in [33], reaction steps involving H and methyl radicals show
greater sensitivity for rich mixtures at high pressure. Such kinetic effect may thus render the UFL more sensitive to the initiate pressure.

3.3 Maximum rate of pressure rise

The maximum rate of pressure rise \((dp/dt)_{\text{max}}\) is a commonly examined parameter for explosion characteristics evaluation and used in deflagration index determination as in several previous studies \([49, 50]\). The results of \((dp/dt)_{\text{max}}\) as a function of DME concentration at different initial pressures are shown in Fig. 7. It can be seen that, the relation between \((dp/dt)_{\text{max}}\) and \(C_{\text{DME}}\) is very similar as that of \(p_{\text{max}}\) as a function of \(C_{\text{DME}}\). The result indicates that the pressure rises more abruptly at higher initial pressure. While for the same initial pressure, the value of \((dp/dt)_{\text{max}}\) is larger near the stoichiometric condition.

It is noteworthy that the rate of pressure rise reaches its maximum value at a slightly higher concentration of approximately 7.5 % \((\phi = 1.159)\) than the stoichiometric condition \((\phi = 1)\), with a mean value of 46.09 MPa/s. Although this behavior is similar to that for the natural gas (NG)-air mixture observed in Zhang et al. \([29]\) (with an average value of 18.86 MPa/s at the NG concentration of 10.5 % or \(\phi =1.117)\), yet the pressure increases more abruptly in DME-air than in NG-air mixtures.

3.4 Laminar burning velocity

Laminar burning velocity \((S_L)\) is a unique property of a combustible mixture, indicating its reactivity and exothermicity in a given diffusive medium. Since it contains the physico-chemical information of the mixture, many premixed flame phenomena, e.g., extinction, flash back, blow-off, and turbulent flame propagation, can be characterized with \(S_L\) being a reference
parameter [28]. In this study, the laminar burning velocity is computed through two different methods. The first one uses the PREMIX module of the CHEMKIN-II. The PREMIX code adopts a hybrid time-integration/Newton-iteration technique to solve the steady-state mass, species and energy conservation equations for a freely propagating flame. It has been widely used in many previous studies [21, 51-54]. In this study, 1200 grid points are imposed in the PREMIX calculations to assure a fully converged prediction. Also a small time-step $\Delta t = 5.0 \times 10^{-7}$ sec is used for the computation. The present PREMIX calculation is coupled with the reaction scheme [14] involving 46 species and 263 reactions. This reaction mechanism was also used previously by Chen et al. [21] to perform PREMIX calculations of the laminar burning velocities for DME/CH$_4$/air mixtures. The mechanism was verified by Chen et al. [21] by comparing measured laminar burning velocities from experiment with calculations and the result shows reasonable agreement with the largest difference less than 10%. The second method considers a mathematical model proposed by Dahoe et al. [31, 32], in which the laminar burning velocity depends on $p_{\text{max}}$ and $dp/dt$. $S_L$ calculated by this model was also used in our previous study of NG-air mixtures [29]. The model gives the following expression:

$$S_L = \frac{1}{(p_{\text{max}} - p_0)^{1/3}} \left( \frac{4\pi}{3V} \right)^{1/3} \left( \frac{p_0}{p} \right)^{1/3} \left( 1 - \left( \frac{p_0}{p} \right)^{1/\gamma} \frac{p_{\text{max}} - p}{p_{\text{max}} - p_0} \right)^{-2/3} \frac{dp}{dt}$$

(1)

where $V$ is the vessel volume, $p$ and $p_0$ are the actual pressure and initial pressure, $\gamma$ the adiabatic coefficient of the unburned gas. $S_L$ is determined by a fitting method proposed by Dahoe, in which $S_L$ is calculated by fitting the pressure history measurement (i.e., actual pressure $p$ and $dp/dt$). A pressure ($p$)- laminar burning velocity ($S_L$) curve is then obtained. Afterwards, $S_{L,0}$ at the reference pressure (i.e., 100 kPa) can be determined by the extrapolate data from a linear curve fit of $p$-$S_L$. [55-57]. $S_L$ is calculated at a flame radius greater than 6 mm to avoid the effect
associated to the spark ignition [58], so the result can be considered as an ideal spherical flame propagating outward.

The laminar burning velocity of DME-air mixtures at different equivalence ratios under 100 kPa determined using the two aforementioned techniques are shown in Fig. 8. The reported results by Qin and Ju [33] and Daly et al. [4] are also included in the same figure for comparison. As shown in Fig. 8, it appears that the computed laminar burning velocity from Eq. (1) agrees reasonably well with the PREMIX simulation. The largest difference between these two sets of data is 42.93 % at the fuel rich condition at 100 kPa. At this condition however, the results from Eq. (1) are very close to the experimental data reported by Qin and Ju [33]. Overall, one can argue that the above comparison shows no significant difference for computing the laminar burning velocity using Eq. (1) and the PREMIX code. Similar comparisons of the computed laminar burning velocity of DME-air mixtures at different equivalence ratios with initial pressures of 80 kPa, 60 kPa and 40 kPa are also shown in Fig. 9. Again, a reasonable agreement between the two results still holds.

Figures 8 and 9 also indicate a decreasing trend of $S_L$ with the increase of initial pressure, e.g., $S_L$ is found to be 61.52 cm/s at 40 kPa which is larger than 48.40 cm/s at 100 kPa at the same composition of $C_{DME} = 7.5 \%$. The behavior of decreasing trend of $S_L$ with the increase of initial pressure is caused by the increasing density, $\rho_u$, with increasing pressure. As demonstrated by Law [28], the eigenvalue for flame propagation is $S_L = f^0/\rho_u$ (where $f^0$ and $\rho_u$ are the mean laminar burning flux and density, respectively). By increasing pressure, $f^0$ increases. It demonstrates that the increase in density with pressure dominates over the retarding effect of $S_L$. 
3.5 Flame radius

The flame radius, \( r_f \), is also calculated through the equation proposed by Dahoe et al. [31, 32] as follows:

\[
\frac{r_f}{r_a} = \left( \frac{3V}{4\pi} \right)^{1/3} \left[ 1 - \left( \frac{P_0}{p} \right)^{1/7} \left( \frac{p_{\text{max}} - p}{p_{\text{max}} - P_0} \right) \right]^{1/3}
\] (2)

where \( r_f \) is the flame radius, \( r_a \) the radius of the vessel and \( \bar{r} \) the dimensionless radius of burned gas. The typical results for stoichiometric DME-air mixtures at different initial pressures are shown in Fig. 10. It can be seen that the flame radius increases just after the time of 0.02 sec, and it increases rapidly until it reaches the wall of the spherical chamber. This process is established as the pressure rise stage. Figure 10 also shows that at the same given time, the dimensionless radius of the flame is relatively greater (i.e., the flame propagates to a longer distance at the same time) at lower initial pressure, which is due to the higher burning velocity.

4 Concluding remarks

This paper presents a detailed investigation on the explosion characteristics (i.e., maximum explosion pressure, flammability limits, maximum rate of pressure rise) and combustion properties (i.e., laminar burning velocity, flame radius) of DME-air mixtures. Experiments are performed by systematically measuring the pressure evolutions in a standard 20-L explosion spherical vessel.

The present measurement shows that the variation between \( p_{\text{max}} \) and DME concentration \( (C_{\text{DME}}) \) exhibits a typical inverse “U” shaped behavior, and \( p_{\text{max}} \) reaches its peak value when its equivalence ratio is slightly larger than 1. It is found from the present measurement that \( p_{\text{max}} \)
decreases as the initial pressure goes down. The flammability region is found to be from 3.5 %
to 19 % of DME by volume at the ambient condition. As the initial pressure decreases from 100 kPa to 40 kPa, the LFL varies slightly and shows little sensitivity to the initial pressure, while the UFL exhibits a more significant drop. The experimental data also show that the explosion pressure rises more abruptly at higher initial pressure. The relation between \((dp/dt)_{max}\) and \(C_{DME}\) is found to be very similar to that of \(p_{max}\) as a function of \(C_{DME}\). Laminar burning velocity was also estimated using both the PREMIX simulation and a mathematical model based on the measured pressure evolution, and a satisfactory agreement is found between those results, especially for \(C_{DME} \leq 9.5\%\). A decreasing trend of \(S_L\) is observed with the increase of initial pressure. This is due to the resulting increase in density with pressure causing the decreasing the observed retarding effect of \(S_L\). Finally, the calculated dimensionless radius of the flame from the pressure history is found to be smaller at higher initial pressure.

Acknowledgments

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Tables

Table 1 Mixture compositions for the experimental tests, along with maximum explosion pressure $p_{\text{max}}$, corresponding combustion time $t_c$, and adiabatic pressure $p_{\text{ad}}$

Table 2 Flammability limits of DME-air at different initial pressures
Table 1

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**Figure captions**

Fig. 1  The 20-L explosion spherical vessel (1 = DME, 2 = air).

Fig. 2  Determination of the maximum explosion pressure and the combustion time from a typical experimental pressure history.

Fig. 3  $p_{\text{max}}$ as a function of DME concentration, compared with Mogi and Horiguchi [25] and adiabatic pressure from equilibrium calculations ($p_0 = 100$ kPa). A curve fit of $p_{\text{max}}$ is also shown in the plot.

Fig. 4  $p_{\text{max}}$ as a function of DME concentration, compared with chemical adiabatic pressure from equilibrium calculations at an initial pressure of $p_0 = 80$ kPa. A curve fit of $p_{\text{max}}$ is also shown in the plot.

Fig. 5  $p_{\text{max}}$ as a function of DME concentration, compared with adiabatic pressure from equilibrium calculations at an initial pressure of $p_0 = 60$ kPa. A curve fit of $p_{\text{max}}$ is also shown in the plot.

Fig. 6  $p_{\text{max}}$ as a function of DME concentration, compared with adiabatic pressure from equilibrium calculations at an initial pressure of $p_0 = 40$ kPa. A curve fit of $p_{\text{max}}$ is also shown in the plot.

Fig. 7  Maximum rate of pressure rise as a function of DME concentration for different initial pressures. Curve fits (shown by the solid lines) are also provided to show the trend in the data.

Fig. 8  Comparison of the laminar burning velocity from chemical simulation and experiment at an initial pressure of $p_0 = 100$ kPa, Data from Qin and Ju [33] and Daly et al. [4] are also shown for comparison.
Fig. 9  Comparison of the laminar burning velocity calculated by detailed reaction kinetic simulations and determined from explosion properties: (a) 80 kPa, (b) 60 kPa; and (c) 40 kPa.

Fig. 10  Dimensionless radius of burned DME-air mixtures with an equivalent ratio of $\phi = 1$ at different initial pressures.
Fig. 1

- Air compressor
- Control unit & Electric ignition system
- Data acquisition system
- Vacuum pump
- Sealing cover
- Igniter
- Circulating water export
- Pressure transducer
- Vacuum meter
- Release valve
- D/2=16.84cm
- 

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Fig. 2

Explosion pressure, MPa

Combustion time, $t_c$

$\rho_{\text{max}}$

$(dp/dt)_{\text{max}}$

$C_{\text{DME}}=10\%$, $p_0=100\text{kPa}$
This study

Curve fit

Adiabatic pressure from equilibrium calculations

Mogi and Horiguchi

$P_{\max}$, MPa

DME concentration, % vol.

Fig. 3
This study
Curve fit
Adiabatic pressure from equilibrium calculations

Fig. 4
This study

Curve fit

Adiabatic pressure from equilibrium calculations

$P_{\text{max}}, \text{MPa}$

DME concentration, % vol.

$\rho_0 = 60\text{kPa}$

No Ignition

$\text{Fig. 5}$
This study

Curve fit

Adiabatic pressure from equilibrium calculations

\( P_{\text{max}}, \text{MPa} \)

\( p_0=40\text{kPa} \)

DME concentration, % vol.

Fig. 6
Fig. 7

The graph shows the relationship between the DME concentration, % vol., and the maximum rate of pressure increase, (dp/dt)$_{max}$, MPa/s, at different pressures: 100kPa, 80kPa, 60kPa, and 40kPa. The graph indicates a peak in (dp/dt)$_{max}$ at a certain DME concentration, followed by a decrease. There is a region labeled "No Ignition" where the DME concentration is low and the rate of pressure increase is minimal. The graph suggests that the ignition characteristics are significantly influenced by the DME concentration and the pressure conditions.
Fig. 8
Fig. 9: Plots showing the relationship between DME concentration (%) and SL (cm/s) at three different pressures: (a) 80 kPa, (b) 60 kPa, and (c) 40 kPa. The red squares represent the data from this study, while the black line represents the PREMIX model predictions.
Fig. 10