#### Fuel 157 (2015) 56-63

Contents lists available at ScienceDirect

### Fuel

journal homepage: www.elsevier.com/locate/fuel

## Explosion behavior of methane-dimethyl ether/air mixtures

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#### HIGHLIGHTS

#### GRAPHICAL ABSTRACT

- Effect of DME addition in promoting the ignition of methane/air mixture is investigated.
- Correlations to evaluate the dimensionless pressure of CH<sub>4</sub>-air and DME-air mixtures with initial pressure are given.
- Calculation of the laminar burning velocity by using both a theoretical model and the CHEMKIN-PREMIX simulation.

#### ARTICLE INFO

Article history: Received 14 January 2015 Received in revised form 14 April 2015 Accepted 22 April 2015 Available online 4 May 2015

Keywords: Dimethyl ether addition Maximum explosion pressure Maximum rate of pressure rise Flammability limits Laminar burning velocity



#### $A \hspace{0.1in} B \hspace{0.1in} S \hspace{0.1in} T \hspace{0.1in} R \hspace{0.1in} A \hspace{0.1in} C \hspace{0.1in} T$

In this study, the effect of dimethyl ether (DME) addition on the explosion of methane/air mixture is investigated. In particular, the explosion and deflagration parameters of various CH<sub>4</sub>-DME/air mixtures are systematically studied. Those parameters include flammability limits, maximum explosion pressure,  $p_{max}$ . maximum rate of pressure rise  $(dp/dt)_{max}$ , and laminar burning velocity S<sub>L</sub>. In general, the experimental results indicate that both  $p_{\text{max}}$  and  $(dp/dt)_{\text{max}}$  increase with increasing DME content in the total fuel. Simple correlations to evaluate the dimensionless pressure ( $\bar{p}$ ) of CH<sub>4</sub>-air and DME-air mixtures with an initial pressure of 100 kPa are developed and given respectively by  $\bar{p} = 1/[2.81839 + 0.22424\gamma_{CH4} - 0.22422\gamma_{CH4} - 0.2242\gamma_{CH4} - 0.224\gamma$ 2.14347*ln*( $\chi_{CH4}$ )] and  $\bar{p} = 1/[1.04153 + 0.12637\chi_{DME} - 0.94532$ *ln* $(<math>\chi_{DME}$ )] where  $\chi$  is the volume fraction of the fuel. The experimental results also indicate that for lean  $CH_4$  mixtures, the relationship between  $p_{max}$ and DME concentration exhibits an inversely "U-shaped" curve. In contrast, an exponential decay of  $p_{max}$ with increasing DME concentration is observed for rich CH<sub>4</sub> mixtures. By adding DME into the CH<sub>4</sub>-air mixture, both the lower and upper flammability limits go down. The maximum amount of the total fuel for the binary blend (CH<sub>4</sub> plus DME) below which the mixture can be initiated is approximately 15–16%. Lastly, a good agreement is found in the determination of the laminar burning velocity  $S_1$  using both a theoretical model and the CHEMKIN-PREMIX simulation. For CH<sub>4</sub>-DME/air mixtures, the S<sub>L</sub> near the stoichiometric equivalence ratio  $\phi_{total}$  = 1 is larger than the fuel lean or rich side. It is found that with a slight amount of DME adding into the lean CH<sub>4</sub> mixture, making  $\varphi_{\text{total}}$  closer to stoichiometry, the value of  $S_{\text{L}}$ increases. However, with further addition of DME into lean CH<sub>4</sub> mixture, or DME adding into rich CH<sub>4</sub> mixture, only a decreasing behavior of  $S_L$  is observed.

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#### 1. Introduction

Alternative fuels with the properties of high-efficiency and lowemission combustion, have received particular interests because of the rapid increase in energy consumption and increasingly stringent emission regulations. Among them, natural gas (NG) is one of the most widely used alternative fuels for automobiles and has long been considered as a promising alternative fuel due to its favorable chemical characteristics, such as: high H/C ratio, large octane number, and especially its low emissions [1-3]. Methane CH<sub>4</sub> as an environmental-friendly fuel and the main component of NG produces less carbon dioxide for each unit of heat released, but more heat per mass unit than other complex hydrocarbons. Nonetheless, methane has some drawbacks regarding its combustion properties, e.g., long ignition delay time, low flame speed, low ignitability and narrow flammability limit range. All of these pose great challenges for its wide utilization in combustion engines [4]. However, using more reactive fuel additives, the ignition and combustion performance of methane could be greatly enhanced. From studies conducted by Dagaut [5,6] and Yao et al. [7,8] on the detailed chemical mechanism for low and high temperature DME oxidation and the effect of DME addition to methane for homogeneous charge compression ignition (HCCI) engines, respectively, DME has shown promise as an effective promoter of high temperature methane ignition. Due to an increasing interest in using NG in the automotive industry, a thorough understanding of the fundamental explosion and combustion characteristics of DME-added mixtures is therefore important for developing advanced, NG-based, combustion engines and corresponding operating strategies [4].

Fundamental combustion properties, such as laminar flame speed and Markstein length, have been extensively studied in the past for methane- [9–11] and DME-air mixtures [12–18]. Many studies have been performed on CH<sub>4</sub>/H<sub>2</sub> or CH<sub>4</sub>/DME binary fuel blends regarding the ignition delay time [4,19–22], internal combustion engine ICE performance [23-25], and laminar flame speed [26-28]. The effects of DME addition on the high temperature ignition and burning properties of methane-air mixtures were also studied experimentally and numerically [19]. Premixed and nonpremixed ignition of methane/DME binary fuel blends with hot air has been studied through numerical simulation with detailed chemistry and various thermodynamic as well as transport properties [4].

While the combustion characteristics of methane mixtures with DME addition have been studied extensively, comparatively little explosion safety data, e.g., maximum explosion pressure,  $p_{max}$ , maximum rate of pressure rise  $(dp/dt)_{max}$ , flammability limits, and laminar burning velocity  $S_{\rm L}$ , are currently available. In fact, the explosion hazard of CH<sub>4</sub>-DME mixtures, within storage infrastructures, is high due to the large destructive energy release associated with the combustion phenomenon. Therefore, in this study, experiments are performed systematically to address the explosion safety problems of CH<sub>4</sub>-DME/air mixtures by recording overpressure histories at different composition of CH<sub>4</sub> and DME in a standard 20-L spherical vessel and analyzing various derived explosion parameters. The data obtained in this study can contribute to a better understanding of the explosion behavior of CH<sub>4</sub>–DME/air mixtures.

#### 2. Experimental details

Measurement of the explosion parameters in CH<sub>4</sub>-DME/air mixtures were carried out in a standard 20-L explosion spherical vessel according to the international standard ISO6184-1. A schematic of the apparatus is shown in Fig. 1. This facility was used previously for the same type of measurement for other gaseous fuels (e.g., natural gas) and detailed information of the experimental details can be found in [29]. In brief, the 20-L explosion spherical

Circulating water export 2 3 Fig. 1. The 20-L explosion spherical vessel (1 = DME, 2 = CH<sub>4</sub>, 3 = air). vessel consists of an explosion chamber, an electric ignition sys-

tem, a control unit, a data acquisition system, a release valve, a vacuum pump and an air pump. A high-voltage electric spark was used to supply the ignition energy as in our previous studies [30–39]. The igniter was mounted at the center of the spherical bomb and a spark energy of 10 J, estimated from  $1/2 \ CV^2$  ("C" and "V" refer the capacitance and voltage, respectively.  $C = 0.1102 \times 10^{-3}$  F, V = 426 V), was delivered by an electric ignition system.

For the explosion experiments, gas concentrations were regulated by the method of partial pressure. The purities of the CH<sub>4</sub> and DME used in this experiment were 99.9% and 99.8%, respectively. The air used in the experiment is of 21% oxygen and 79% nitrogen (by volume). The experiments were performed at initial pressure of 100 kPa and temperature of 298 K. 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 raw values of the explosion pressure and rate of pressure rise. In the present study, at least three shots were repeated at the same initial condition of the experiment, and five or more shots were made for the mixtures near LFL and UFL. Thus, the LFL and UFL were determined if half shots indicated explosion occur.

#### 3. Results and discussion

#### 3.1. Maximum explosion pressure and maximum rate of pressure rise

Samples of pressure traces obtained from experiments are shown in Fig. 2. In Fig. 2,  $p_{\rm max}$  occurs at the peak of the curve, however,  $(dp/dt)_{max}$  represents the steepest part of the pressure curve and hence, the maximum of these parameters do not occur at the same place. To characterize the mixtures,  $\lambda$  is defined as the ratio of DME over the total fuel (i.e., CH<sub>4</sub> plus DME) as follows:

$$h = \frac{C_{\rm DME}}{C_{\rm DME} + C_{\rm CH4}} \tag{1}$$

in which  $C_{CH4}$  and  $C_{DME}$  denote the  $CH_4$  and DME concentration, respectively.  $\lambda$  varies from 0 (pure CH<sub>4</sub>) to 1 (pure DME). Unless specified, the total fuel is at the stoichiometric concentration with air. It can be seen from Fig. 2 that the maximum explosion pressure  $p_{\text{max}}$  increases with  $\lambda$ . It should be noted again that the  $\varphi_{\text{total}}$  (equivalence ratio of the overall fuels over air) is kept to 1 as  $\lambda$  changes. The slope of the pressure history is also observed to become more steep or in other words, the maximum rate of pressure rise (dp/ dt<sub>max</sub> increases as well with increasing  $\lambda$ . Fig. 3 summarizes the



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