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Study on Dimethyl Ether−Air Premixed Mixture Combustion with a Constant Volume Vessel

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Combustion characteristics of dimethyl ether−air premixed mixtures were studied in a constant volume bomb. A two-zone model was proposed for predicting combustion parameters based on the pressure data. For a specified initial pressure, the mixtures around the stoichiometric equivalence ratio give the maximum pressure rise rate, the maximum mass burning rate, the maximum combustion pressure, and the maximum burned gas temperature. The shortest flame development duration and combustion duration occur around the stoichiometric mixture. A small difference in flame development duration and combustion duration within the three low initial pressures suggests that initial pressures of the mixture at low pressures have a small influence on the combustion duration.

Introduction

With increasing concern about possible energy shortages and environmental problems, research on improving engine fuel economy and reducing exhaust emissions has become a major research aspect in combustion and engine development communities. Alternative fuels, usually belonging to clean fuels compared to diesel fuel and gasoline fuel, are beneficial to the slowing of the fuel shortage and reduction of engine exhaust emissions. Dimethyl ether (DME) is the simplest aliphatic ether without carbon−carbon bonds. It has a high oxygen fraction, high cetane number, low combustion noise, and smoke-free combustion.[1−2]

However, for engine application, the low boiling point of DME needs the fuel to be pressurized in the tank and the low heating value of DME needs to increase the fuel injection amount to get the diesel-equivalent power. A previous study showed that the diesel engine could operate on DME if some modifications were made in the fuel pump and fuel tank without modification of the engine and relatively low cost.[3−4]

Up to now, most work on DME was concentrated on the spray characteristics and engine application,[5−6] and a few papers were

reported on flame propagation of the premixed dimethyl ether−air flames.[7−9] The previous works reported the burning velocities of dimethyl ether−air flames, and the analysis was usually made based on the flame photos. Further information on premixed flames of the dimethyl ether−air mixtures needs to be clarified, and this will provide new information for the understanding of dimethyl ether−air combustion or supply the guidance for engine operation.

The objective of this paper is to study the combustion characteristics of dimethyl ether−air premixed mixtures based on the analysis of the mass burning rate (or heat release rate) at low initial pressures by using a constant volume vessel, and a two-zone model is used to calculate the combustion parameters based on the recorded pressure data.

Experimental Section

The experiment was conducted in a constant volume vessel as shown in Figure 1. The combustion bomb is a cuboid type with an inside size of 108 × 108 × 135 mm. The combustible mixture is prepared within the chamber by adding dimethyl ether and air at the specified partial pressures. The mixture is ignited by the centrally located electrodes, and a standard capacitive discharge ignition system is used for producing the spark. In this study, the ignition energy is 45 mJ. The pressure is recorded by a piezoelectric Kistler absolute pressure transducer with a resolution of 0.01 kPa. In the experiments, limited by the structural strength of the constant

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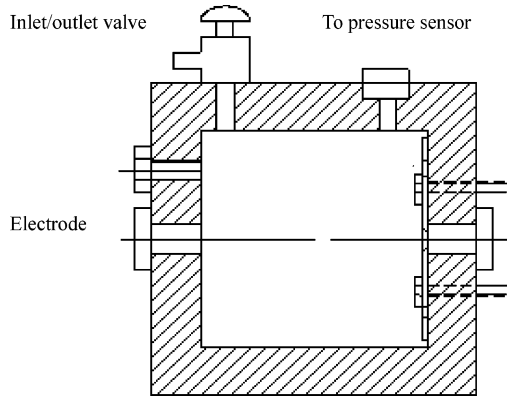
Figure 1. Constant volume combustion bomb.

Table 1. Fuel Properties of Dimethyl Ether

fuel	dimethyl ether
chemical formula	CH_3-O-CH_3
molecular weight (g)	46.07
boiling point (°C)	−24.9
Reid vapor pressure (MPa)	0.51 (20 °C)
liquid density (g/cm³)	0.668
liquid viscosity (cP)	0.15
low-heating value (MJ/kg)	28.43
explosion limit in air (vol %)	3.4−17
ignition temperature (K)	235
stoichiometric air/fuel ratio	9
latent heat of evaporation (kJ/kg)	460 (−20 °C)

volume bomb, the initial pressure is set from 0.08 to 0.15 MPa and the initial temperature is 285 K. Table 1 gives the fuel properties of dimethyl ether. Dimethyl ether is in the gaseous state at room temperature, and the pressure is less than 0.5 MPa; thus, the homogeneous dimethyl ether−air mixture can be prepared in the combustion chamber by regulating the partial pressures of dimethyl ether and air. In the experiments, the constant volume vessel was vacuumed by a vacuum pump; then dimethyl ether was introduced into the constant volume bomb; and its amount was regulated to the desired pressure through a mercury gauge. Finally, the pressure of the vessel was regulated to the initial pressure.

Experiments were conduced at room temperature, and the initial pressures were strictly regulated at the specified initial pressures. A sufficient interval between experiments is used to ensure that the walls cool down. It was noted that the repeated experiments under the same condition showed good consistency, and this made the data usable.

Calculation Model. A two-zone model is proposed for combustion analysis based on the pressure data obtained in the experiments. The spherical flame front divides the combustion chamber into the burned zone and the unburned zone as shown in Figure 2. The symbol p, T, V, and m represent the pressure, temperature, volume, and mass of the chamber gases, respectively, and Q_r is the amount of heat release by fuel combustion. The subscripts u and b represent the unburned and burned states, respectively. After assumptions are made in the model: (1) The gases are regarded as the ideal gases. (2) Complete combustion finishes very rapidly when the unburned charge enters the burned zone. (3) Pressure reaches its equilibrium value instantaneously, and there is no difference between the burned and unburned zones. (4) No gas leakage is occurring, and the gas temperature reaches its respective temperature in the burned and unburned zones. (5) The unburned gases are regarded as the mixture of dimethyl ether and air. (6) Gas properties of unburned and burned gases are the mixture properties calculated by the fraction of the constituted gases.

The mass conservation equation is written as

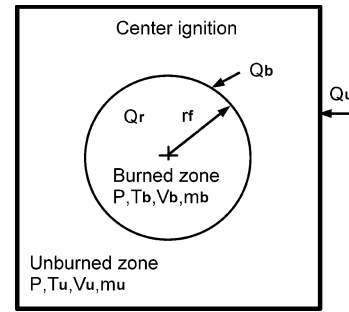$$\frac{dm_u}{dt} = -\frac{dm_b}{dt} \tag{1}$$

Figure 2. Schematic diagram of the two-zone model.

From energy conservation, the following two equations can be established

$$\frac{d(m_u u_u)}{dt} = -P\frac{dV_u}{dt} + \frac{dm_u}{dt}h_u + \frac{dQ_u}{dt} \tag{2}$$

$$\frac{d(m_b u_b)}{dt} = -P\frac{dV_b}{dt} + \frac{dm_b}{dt}h_b + \frac{dQ_b}{dt} + \frac{dQ_r}{dt} \tag{3}$$

Because the same pressure is considered in both the burned and unburned zones, from the ideal gas assumption, eq 4 can be established

$$P = \frac{m_b R_b T_b}{V_b} = \frac{m_u R_u T_u}{V_u} \tag{4}$$

From the above 4 equations, the following equations can be derived:[10]

$$\frac{dT_u}{dt} = \frac{\dfrac{T_u}{P}\dfrac{dP}{dt} + \dfrac{\dfrac{dQ_u}{dt}}{m_u R_u}}{\dfrac{1}{R_u}\dfrac{du_u}{dT_u} + 1} \tag{5}$$

$$\frac{dm_b}{dt} = \frac{\dfrac{dQ_b}{dt} + \dfrac{dQ_r}{dt} + \left(m_u R_u \dfrac{dT_u}{dt} - PdV\right)\left(\dfrac{1}{R_b}\dfrac{du_b}{dT_b} + 1\right) - V\dfrac{dP}{dt}\left(\dfrac{1}{R_b}\dfrac{du_b}{dT_b} + \dfrac{m_b}{V}\dfrac{du_b}{dT_b} + \dfrac{V_u}{V}\right)}{(u_b - u_u) + \left(\dfrac{R_u}{R_b}T_u - T_b\right)\dfrac{du_b}{dT_b}} \tag{6}$$

$$\frac{dV_b}{dt} = V_u\left(\frac{1}{m_u}\frac{dm_u}{dt} - \frac{1}{T_u}\frac{dT_u}{dt} + \frac{1}{p}\frac{dP}{dt}\right) + \frac{dV}{dt} \tag{7}$$

Heat-Transfer Calculation. The model takes into account both convective heat transfer and radiation. The coefficient of convective heat transfer is derived from the plate−plate convective heat-transfer correlation as follows:

$$\alpha = C\frac{\lambda}{L_c}R_e \tag{8}$$

in which λ is the gas conductive coefficient in kW m^{-2} K^{-1}, L_c is the characteristic length, and R_e is the Reynolds number, where $R_e = \rho v L_c/\mu$, with v being the velocity in m/s and μ being the viscosity.

(10) Ma, F. H. Fundamental study of premixed turbulent combustion. Ph.D. Dissertation, Xian Jiaotong University, Xian, China, 1997.

The radiant heat-transfer flux, q_r, is calculated by

$$q_r = K\sigma(T^4 - T_i^4) \tag{9}$$

in which σ is the Boltzmann constant, $\sigma = 5.67 \times 10^{11}$ kW m^{-2} K^{-4}.

Thus, the transient heat transfer to the wall, dQ_u/dt, and the transient heat transfer from burned gas to unburned gas, dQ_b/dt, are determined by

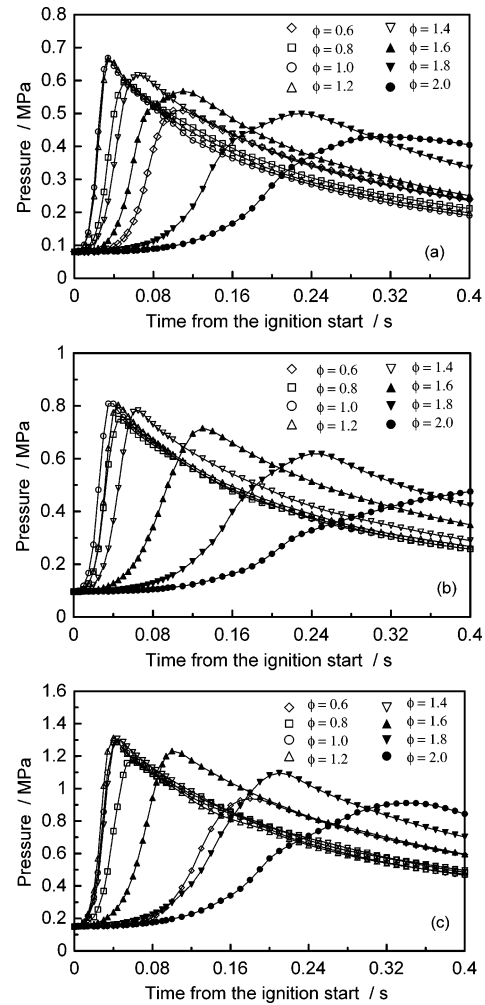$$\frac{dQ_u}{dt} = A[\alpha(T_u - T_w) + K\sigma(T^4 - T_w^4)] \tag{10}$$

$$\frac{dQ_b}{dt} = A_f[\alpha(T_b - T_u) + K\sigma(T_b^4 - T_u^4)] \tag{11}$$

This is the typical Annand's heat-transfer formula. Here, the constant K uses the value of 1.5; A is the wall surface area; and A_f is the spherical flame front area, which can be calculated by $A_f = (4\pi)^{1/3}(3V_b)^{2/3}$. T_u and T_b are the gas temperature for unburned and burned zones, while T_w is the wall temperature.

In the model, the gas temperatures are assumed to be uniform in the unburned and burned zones; thus, the no temperature gradient was considered in the model. With respect to the model calculation, dP/dt is obtained from the pressure data in the experiments and dV/dt is 0 for the constant volume bomb. Internal energy and gas constant of mixtures, u_b, u_u, R_b, R_u, du_b/dT_b, and du_u/dT_u, are calculated using the formula given in the literature,[10] according to the fraction of each species. Thus, the unknown variables in these thermodynamic equations are m_b, T_b, and T_u. The initial unburned gas temperature T_b uses the adiabatic flame temperature T_{ad}, using the fourth-order Runge−Kutta scheme, and the m_b, T_b, T_u, and burning rate, dm_b/dt, can be obtained. During the combustion process, gas compositions and properties are calculated through chemical equilibrium with 11 species and 7 equations.[11]

Results and Discussions

Figure 3 shows the combustion pressure curves under different equivalence ratios for three initial pressures. For a specified initial pressure, the mixtures around the stoichiometric equivalence ratio give the maximum rate of pressure rise and the maximum value of combustion pressure. The shortest duration from the ignition start to the maximum pressure arriving is presented, indicating the fastest flame speed around the stoichiometric equivalence ratio. When the mixtures become rich or lean, the rate of pressure rise decreases and the period from the ignition start to the maximum pressure arriving increases. This reveals the decrease of the mixture flame propagation speed. In the case of lean mixture combustion, the fuel available volumetrically and combustion temperature will decrease, leading to the decrease in the reaction rate of the dimethyl ether−air mixture. In the case of rich mixture combustion, the insufficiency of oxygen decreases the reaction rate of the dimethyl ether−air mixture. For lean mixture combustion, the increase in the combustion duration will lead the increase in heat loss to the wall; meanwhile, the total heat value of the mixture will decrease. These two factors are considered to contribute to the decrease of the maximum combustion pressure for lean mixture combustion. For rich mixture combustion, the incomplete combustion as a result of lacking oxygen and the increase in the heat loss to the wall as a result of increasing combustion duration are considered to contribute to the decrease of the maximum combustion pressure. This phenomenon becomes more obvious in the case of richer
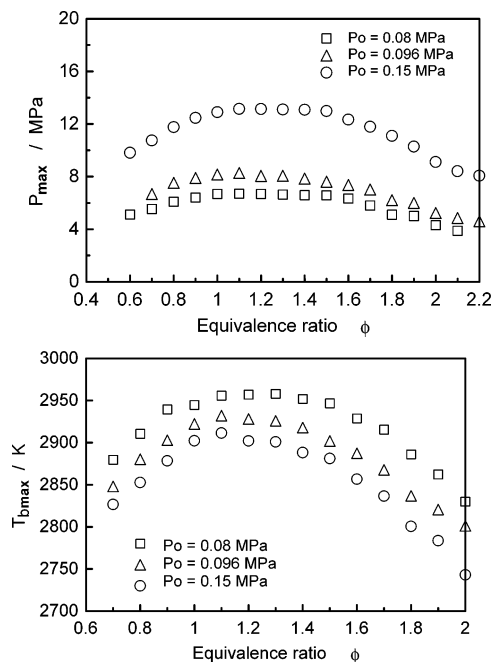
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Figure 3. Pressure history at different equivalence ratios and initial pressures. (a) $P_0 = 0.08$ MPa, $T_0 = 285$ K; (b) $P_0 = 0.096$ MPa, $T_0 = 285$ K; and (c) $P_0 = 0.15$ MPa, $T_0 = 285$ K.
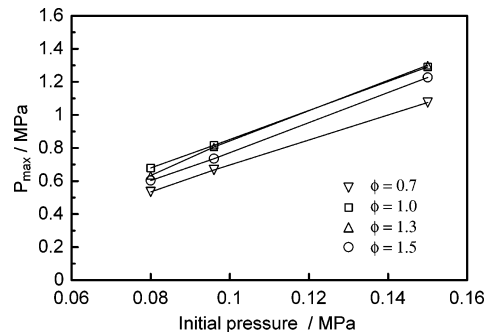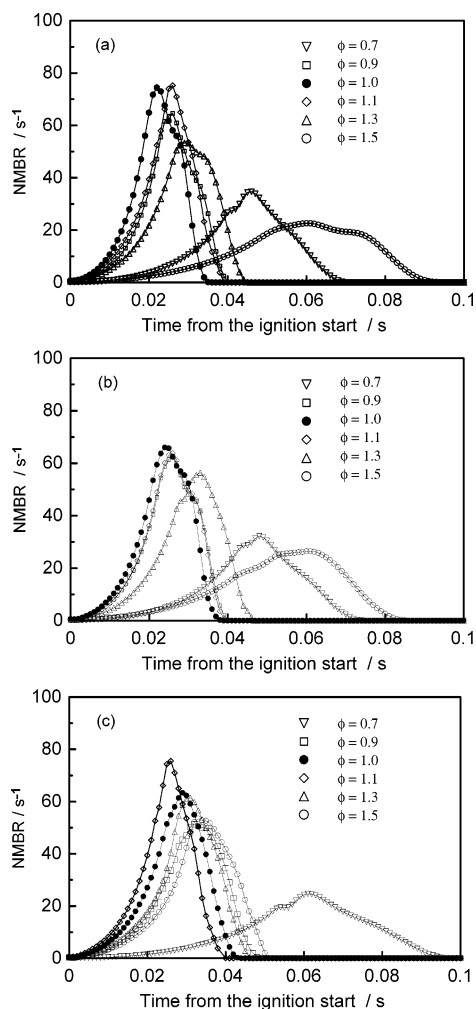

Figure 4. Maximum pressures versus initial pressures.

or leaner mixtures. The maximum combustion pressures of dimethyl ether−air combustion versus the initial pressures under the different equivalence ratios are plotted in Figure 4. Better linear correlation between the maximum combustion pressure and the initial pressure is demonstrated, and this indicates that the maximum combustion pressure increases linearly with the increase of the initial pressure for dimethyl ether−air premixed combustion. The study also reveals that the slope of the maximum combustion pressure to the initial pressure keeps the same value regardless of the equivalence ratios, and this indicates that the same increase in the maximum combustion pressure will be given at the same initial pressure, increasing regardless of equivalence ratios.
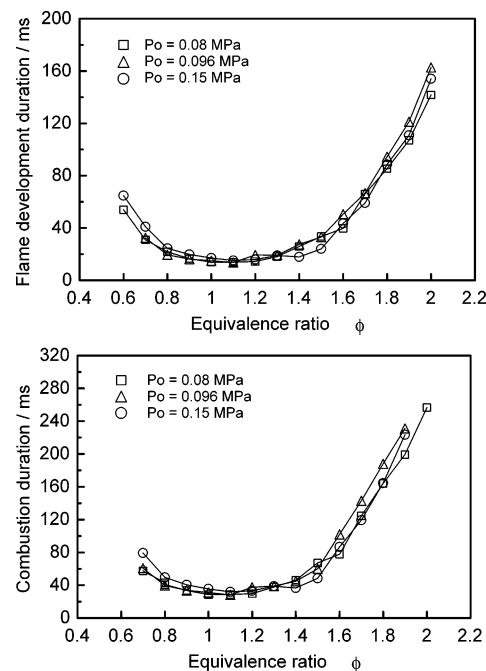
Figure 5. Maximum pressures and maximum mean temperature of burned gases versus equivalence ratios.

Figure 6. Normalized heat release rate at three initial pressures. (a) $P_0 = 0.08$ MPa, $T_0 = 285$ K; (b) $P_0 = 0.096$ MPa, $T_0 = 285$ K; and (c) $P_0 = 0.15$ MPa, $T_0 = 285$ K.

Figure 5 gives the maximum combustion pressure P_{max} and the maximum mean burned gas temperature $T_{b,max}$ versus the

Figure 7. Combustion duration versus equivalence ratios.

equivalence ratios. Here, $T_{b,max}$ is calculated by the two-zone model. For a specified initial pressure, P_{max} and $T_{b,max}$ give the maximum value at the equivalence ratios around the stoichiometric equivalence ratio, and the equivalence ratio at P_{max} and $T_{b,max}$ will move to the rich mixture side while increasing the initial pressure. This suggests that increasing the initial pressure can improve the combustion at rich mixture sides. These are consistent with the moving of the laminar burning velocity of dimethyl ether−air mixtures, because the laminar burning velocity will move to the rich mixture side while increasing the initial pressure.[12]

In this paper, the normalized mass burning rate is defined as $1/m \, dm_b/dt$ (or is designated by NMBR), where m is the total mass of combustible gases and m_b is the mass of burned gases. The NMBR rate is calculated from the proposed two-zone model described above, and this parameter can reflect the burning velocity of the mixture during the combustion process.

Figure 6 shows the NMBR under different equivalence ratios and three initial pressures (0.08, 0.096, and 0.15 MPa). In the cases of initial pressures at 0.08 and 0.096 MPa, the maximum NMBR and shortest combustion duration are presented at the mixtures around the stoichiometric equivalence ratio. When the mixtures become lean or rich, NMBR tends to decrease and combustion duration tends to increase. In the case of an initial pressure at 0.15 MPa, the maximum NMBR and shortest combustion duration are demonstrated at the equivalence ratio larger than the stoichiometric equivalence ratio ($\phi = 1.1$), indicating that the maximum NMBR moves toward the rich mixture side while increasing the initial pressure. These can also be explained by the behaviors of the laminar burning velocity with a variation of the initial pressure.[12]

The flame development duration is defined as the duration from the ignition start to the timing of 10% of the mixture burned, and the combustion duration is defined as the duration from the ignition start to 90% of the mixture burned.[13] Figure

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7 gives the flame development duration and combustion duration versus equivalence ratios. The shortest flame development duration and shortest combustion duration occur at mixtures near the stoichiometric mixture (in the range between $\phi = 1.0$ and 1.2). For lean mixture combustion (equivalence ratios are less than 1.0), the flame development duration and combustion duration increase while decreasing the equivalence ratios. For rich mixtures with equivalence ratios larger than 1.2, the flame development duration and combustion duration increase while increasing the equivalence ratios. When the equivalence ratios are larger than 1.5, the flame development duration and combustion duration show a remarkable increase when further increasing the equivalence ratios. The study reveals a small difference in the flame development duration and combustion duration within the three low initial pressures, and this suggests that initial pressures of the mixture at low pressures have a small influence on the combustion duration.

Conclusions

(1) For a specified initial pressure, the mixtures around the stoichiometric equivalence ratio give the maximum rate of pressure rise, the maximum mass burning rate, the maximum combustion pressure, the maximum burned gas temperature, and the shortest duration from the ignition start to the timing of the maximum combustion pressure.

(2) The shortest flame development duration and shortest combustion duration occur at mixtures near the stoichiometric mixture. A small difference in flame development duration and combustion duration with a variation of initial pressures are observed, and this suggests that the initial pressure of the mixture at low pressure has a small influence on the combustion duration.

Nomenclature

A = Wall area (m^2)

A_f = Flame front area (m^2)

h = Enthalpy (J)

L = Molar number of air

L_c = Characteristic length (m)

m = Mass of gases (g)

NMBR = Normalized mass burning rate (s^{-1})

P = Gases pressure (Pa)

P_o = Initial mixture pressure (MPa)

q_r = Radiant heat-transfer flux (W/m^2)

dQ_b/dt = Heat-transfer rate from burned gas to unburned gas (J/s)

Q_r = Amount of heat release by fuel combustion (J)

dQ_u/dt = Heat-transfer rate from the unburned zone to wall (J/s)

R = Gas constant (J g^{-1} K^{-1})

R_e = Reynolds number

T = Gas temperature (K)

T_w = Wall temperature (K)

u = Internal energy (J)

ν = Velocity (m/s)

V = Volume (m^3)

t = Time (s)

ϕ = Equivalence ratio

α = Heat-transfer coefficient (W m^{-2} K^{-1})

λ = Gas-conductive coefficient (W m^{-2} K^{-1})

ρ = Gas density (kg/m^3)

σ = Boltzmann constant

μ = Viscosity (kg m^{-1} s^{-1})

Subscripts

b = Burned gases

u = Unburned gases