Fuel 210 (2017) 729–737

Contents lists available at ScienceDirect

Fuel

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

Full Length Article

Determination of the explosion characteristics of methanol – Air mixture in a constant volume vessel

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ARTICLE INFO

Keywords:
Methanol
Explosion
Burning velocity
Explosion index
Closed vessel
Combustion

ABSTRACT

Methanol is now an important alternative fuel. A new multizones model was implemented to experimentally determine the fundamental explosion characteristics of method-air mixtures using a closed vessel. Experiments of the methanol-air mixtures at different initial conditions of temperature, pressures and equivalence were undertaken in a closed spherical vessel with central ignition. Firstly, methodology to determine the key explosion characteristics by integrating the experiments and multizones model is presented. Maximum explosion pressures as a function of equivalence ratio at different initial pressure and temperatures were measured and presented. A linear relationship between the maximum explosion pressure and initial pressure was found to exist. The maximum rate of pressure rise (dP_{max}/dt) and explosion or deflagration index (K_G) were found to increase with increase in the initial pressures but decreased with increase in initial temperature. The 10% explosion delay time ($ED^{10\%}$) was found to increase with increasing maximum explosion pressures. The laminar burning velocity (Su) was found to have a linear relationship with maximum explosion pressure, dP_{max}/dt and K_G. Onset of cellularity was found to significantly affect the rate of pressure rise, maximum rate of pressure rise and burning velocity of methanol-air mixtures.

1. Introduction

The importance of alcohols or bio-alcohols has been growing recently due to their potential for reducing tail pipe emissions [1–6]. In the literature, methanol has attracted significant attention as an alternative fuel because it can be synthesized from a wide range of feedstocks [7]. Typically, methanol as a fuel has lower energy content and high hygroscopicity, presenting storage and transportation challenges [8].

Methanol is a flammable liquid fuel, and has high evaporation characteristics which can generate exploding vapors during leakage under high temperature conditions leading to explosions and disasters [8–12]. Therefore, the safety issue claims high concern over the fuel utilization, storage and transportation, calling for investigation on the explosion characteristics to assess the potential explosion hazard of methanol.

In the literature, explosion behaviour of methanol-air mixtures has not attracted much attention. There is still a lack of clear understanding on the key fundamental explosion characteristics of methanol-air mixtures such as its explosion pressures (Pex), explosion delay (θ_{ex}) explosion pressure rise (dP/dt), maximum rate of pressure rise (dP_{max}/dt), explosion or deflagration index 'K_G', and laminar burning velocity (S_u) [9,13]. These fundamental properties are essentially needed for the prevention of explosions in domestic and industrial or process plant environments for "constructive explosion protection" [9,13]. This is needed to correctly determine and assess the explosion risks, to avoid explosion disasters from flammable fuels during storage, transportation and manufacturing, failures of chemical and petrochemical plants, failure of high pressure vessels, fuels leaks in buildings, fuel tank cleaning of planes and ships [14]. These important characteristics are also very important for vent area design [9,15,16] and explosion transmission between interconnected vessels [9,17,18]. Also, laminar burning velocity data is importantly needed for calculations of the explosion protection, fuel tank venting, engine design, modelling of turbulent combustion, and validation of chemical kinetics mechanism [8–9,19–21]. The detailed knowledge of these characteristics provides insight into such properties as heat release rates, flammability limits, propagation rates, quenching and emission characteristics [19].

In the literature, the main focus on the methanol fuel has been on the development of its kinetic reaction mechanism [22–26], burning velocity measurements [19,27–31], and its performance and emission characteristics in engines [32,33]. Recently, Mitu and Brandes [9] have undertaken experimental study of the explosion characteristics of methanol-air mixtures in a 5 litre stainless steel spherical vessel with central ignition. They have determined the e explosion pressures, the rate of pressure rise as a function, deflagration index, and laminar

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http://dx.doi.org/10.1016/j.fuel.2017.09.004
Received 21 July 2016; Received in revised form 4 September 2017; Accepted 5 September 2017

burning velocity as a function of the fuel/ air ratio at different initial temperatures and pressures. They observed the dependence of these key characteristics on the initial pressures but within the temperature range investigated, temperature dependence could not be established [9].

Chang et al. [34] in 2009 investigated the fire and explosion characteristics of methanol and toluene mixtures approached to minimum oxygen concentration. They have measured for the varied minimum initial oxygen concentration (MOC) the critical fire and explosion properties, for the explosion sensitivity (lower explosion limit (LEL), upper explosion limit (UEL)), maximum explosion pressure (P_{max}), maximum rate of explosion pressure rise $(dP\,dt^{-1})_{max}$ and explosion damage degree (gas or vapor deflagration index (K_g)/St Class). Zhang et al. [35] measured the peak combustion pressure, flame development duration and combustion duration for methanol – air mixtures inside the closed vessel. They observed that combustion pressure, the mass burning rate, and the burned gas temperature reach minimum value at an equivalence ratio of 1.1. They also observed that the flame development duration, the combustion duration and the peak combustion pressure decrease with the increase of the initial temperature, while the maximum burned gas temperature increases with the increase of the initial temperature. The peak combustion pressure and temperature increase with the increase of the initial pressure. The flame development duration and combustion duration increase with the increase of the dilution ratio, while the peak combustion pressure and temperature decrease with the increase of the dilution ratio. Recently, Li et al. [8] measured the explosion characteristics of five alcohols (ethanol, 1-butanol, 1-pentanol, 2-pentanol and 3-pentanol. They observed that the peak explosion pressure is increased with the decrease of temperature and increase of pressure. Maximum rate of pressure rise is insensitive to the temperature variation, while it significantly increases with the increase of initial pressure.

The aim of this paper is to present in detail the explosion characteristics of methanol-air mixtures measured in a closed vessel at Oxford engine research group is presented. Firstly, a brief description of the novel multizones model to model the deflagration of methanol-air mixtures in a closed vessel is presented. Secondly, a brief description of the experimental facility to undertake experiments at elevated initial temperatures, pressures and different equivalence ratios is presented. Next, the methodology to determine the key explosion parameters using the multizones model and experimental data is presented. Subsequently, key explosion characteristics of methanol – air mixtures such as maximum pressure, maximum rate of pressure rise, maximum explosion delay, deflagration index and burning velocity were determined and presented at different initial temperatures, pressures and equivalence ratios. Finally, the effects of cellularity are determined and presented.

2. Multizones model

A novel multizones model for the premixed laminar combustion inside a closed vessel, developed by the present author [19–21,36], is used in the present work. The multizones model has been considered as the most comprehensive model for the laminar premixed combustion inside closed vessel [37,38]. The assumptions used, derivation and detailed methodology of applying the model to closed spherical vessel have been presented in the previous work [19–21,36]. However, a brief description about it is included in the present work to give a completeness of the measurement procedures implemented. The multizones model was derived for the laminar combustion of the premixed fuel-air mixture of negligible flame thickness. In the multizones model, the explosion starts at the centre of the spherical vessel, propagating outwardly and finally ending at the vessel walls as shown in Fig. 1.

Using the conservation of volume and energy in the vessel, a set of the ordinary differential equations for the rate of change of pressure, burned and unburned gas temperatures for a multiple zones model were derived:

$$\frac{dP}{dt} = \frac{A + B_u + \Sigma B_i}{\Sigma C_i + D} \quad (1)$$

$$\frac{dT_u}{dt} = \frac{-\mathbf{h}\left(\pi\frac{b^2}{2} + \frac{4V}{b}\right)(1-x^{0.5})(T_u-T_w)}{m(1-x)C_{P,u}} + \frac{v_u}{C_{pu}} * \frac{\partial \ln v_u}{\partial \ln T}\left(\frac{A + B_u + \Sigma B_i}{\Sigma C_i + D}\right) \quad (2)$$

where, P is the pressure, t is the time, T is the temperature, $C_{p,u}$ is the specific heat, x is mass fraction burned, V is the total volume, v is the specific volume, $\boldsymbol{h}$ is the heat transfer coefficient, and m is the mass.

$$\frac{dT_{bi}}{dt} = -(1-x)\frac{v_u}{T_u}\frac{\partial \ln v_u}{\partial \ln T_u} * \frac{T_{bi}}{xv_{bi}}\frac{\partial \ln T_{bi}}{\partial \ln v_{bi}} * \frac{v_u}{C_{pu}}\frac{\partial \ln v_u}{\partial \ln T_u} * \frac{\partial \ln v_u}{\partial \ln T_u}\left(\frac{A + B_u + \Sigma B_i}{\Sigma C_i + D}\right) + \frac{v_u}{T_u}\frac{\partial \ln v_u}{\partial \ln T} * \frac{T_{bi}}{xv_{bi}}\frac{\partial \ln T_{bi}}{\partial \ln v_{bi}} * \frac{\mathbf{h}A(1-x^{0.5})(T_u-T_w)}{mC_{P,u}} - \frac{T_{bi}}{xv_{bi}}\frac{\partial \ln T_{bi}}{\partial \ln v_{bi}} \left(x\frac{v_{bi}}{P}\frac{\partial \ln v_{bi}}{\partial \ln P} + (1-x)\frac{v_u}{P}\frac{\partial \ln v_u}{\partial \ln P}\right)\left(\frac{A + B_u + \Sigma B_i}{\Sigma C_i + D}\right) - \frac{T_{bi}}{xv_{bi}}\frac{\partial \ln T_{bi}}{\partial \ln v_{bi}}(v_{bi}-v_u)\frac{dx}{dt} \quad (3)$$

where, $\Sigma(B_i) = B_1 + B_2 + B_3 + \ldots. + B_n$

$$A = \frac{v_u}{C_{P,u}}\frac{\partial \ln v_u}{\partial \ln T_u} * \mathbf{h}A(1-x^{0.5})\frac{(T_u-T_w)}{T_u} \quad (4)$$

$$B_u = (v_u-h_u)\frac{dx}{dt} \quad (5)$$

$$B_i = \left(-v_{bi} + \frac{v_{bi}}{C_{p,bi}T_{bi}}h_{bi}\right)\frac{dx}{dt} \quad (6)$$

$$C_i = x\left(\frac{v_{bi}^2}{C_{pbi}T_{bi}}\left(\frac{\partial \ln v_{bi}}{\partial \ln T_{bi}}\right)^2 + \frac{v_{bi}}{P}\frac{\partial \ln v_{bi}}{\partial \ln P}\right) \quad (7)$$

$$D = (1-x)\left(\frac{v_u^2}{C_{pu}T_u}\left(\frac{\partial \ln v_u}{\partial \ln T_u}\right)^2 + \frac{v_u}{P}\frac{\partial \ln v_u}{\partial \ln P}\right) \quad (8)$$

subscript, u, b, and i indicates the unburned, burned and individual burned zones.

The above model was solved computationally and a *BOMB* program [20,39] was evolved. The methodology adopted to find the solution and development of the *BOMB* program is presented in [20,39]. The *BOMB* program takes the following input: Fuel Type, Composition of Air (O2/N2), Number of Zones, initial temperature, pressure, and equivalence ratio, humidity, residual or diluents. And output the following for the steps of mass fraction burned: explosion pressure, unburned and burned gas temperature in each zone, volume and radius of individual, burned gas products in each zones, flame radius. These outputs are used to determine the experimental measurements of combustion characteristics.

3. Experimental facility used

The premixed constant volume spherical vessel combustion test facility used in the present study is shown in the schematic diagram in Fig. 2. It consists of the following: Combustion vessel and heating system, ignition circuit, gaseous and liquid fuel handling system, and data acquisition system. Fig. 3 shows the details of the spherical combustion test vessel with heating system. The combustion test vessel is a steel spherical vessel (160 mm diameter internal diameter) with two optical access windows and central spark ignition. Tests can be done in this vessel up to the maximum operating pressure of 34 bars. The combustion vessel is placed inside a heating system which is employed to achieve two purposes: testing of the mixture at elevated initial temperatures and the exact mixture preparation of liquid fuels at high temperatures. A temperature of 475 K inside the test vessel can be achieved and maintained using the heating system. The combustion vessel has central ignition with two diametrically opposed electrodes powered by a standard *Lucas* inductive ignition system consisting of coil drive module giving spark energy of about 1 mJ [27], which is more than the minimum ignition energy of the fuels tested on the present