Comparative assessment of the explosion characteristics of alcohol—air mixtures

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Qianqian Li, Yu Cheng, Zuohua Huang[*]

State Key Laboratory of Multiphase Flow in Power Engineering, Xi'an Jiaotong University, Xi'an, 710049, People's Republic of China

ABSTRACT

Explosion characteristics of five alcohol—air (ethanol, 1-butanol, 1-pentanol, 2-pentanol and 3-pentanol) mixtures were experimentally conducted in an isochoric chamber over wide ranges of initial temperature and pressure. The effect of temperature and pressure on the different explosion behaviors among these alcohols with various structures were investigated. Results show 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. Among the 1-, 2-, and 3-pentanol—air mixtures, 1-pentanol has the highest values in peak explosion pressure and maximum rate of pressure rise and 2-pentanol gives the lowest values at the initial pressure of 0.1 MPa. These differences tend to be decreased with the increase of initial pressure. Among the three primary alcohol—air (ethanol, 1-butanol and 1-pentanol) mixtures, a similar explosion behavior is presented at the lean mixture side because of the combined effect of adiabtic temperature and flame propagation speed. At the rich mixture side, 1-pentanol gives the highest values in peak explosion pressure and maximum rate of pressure rise and ethanol gives the lowest values. This phenomenon can be interpretated from the combining influence of heat release and heat loss, *since the flame speeds of ethanol-, 1-butanol-, 1-pentanol—air mixtures are close at rich mixture side.*

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1. Introduction

The interest in bio-alcoholic renewable fuels is increasing because of energy shortages and serious environmental pollution. In the past decades, extensive studies on bio-alcohols suggested that alcohols addition potentially favors to the reduction of emissions, especially the particulate matter (Gautam and Martin, 2000; Gautam et al., 2000; Yucesu et al., 2006; Koc et al., 2009; Ozsezen and Canakci, 2011; Surisetty et al., 2011). Low alcohols like ethanol with high octane number and relatively low cost have been successful in the practical use as the gasoline additives. However, low alcohols still have their disadvantages such as low energy content and high hygroscopicity. This leads to an inconvenient storage and transportation and restricts their wide applications in engines. Meanwhile, low alcohols favor to the knock resistance in the spark ignition (SI) engines but they are bad for compression ignition (CI) engines. Recent study on the higher alcohols indicated that 1-pentanol presents a negative temperature coefficient (NTC)

behavior in the intermediate temperature regime, which indicates their potential of fuels for the CI engines (Heufer et al., 2013). An engine study on the 1-pentanol/diesel blend reported that, compared with pure diesel, the blend exhibited the comparative engine performance, lower particulate emissions, and even better combustion characteristics for the blending ratio of pentanol up to 25% (Campos-Fernandez et al., 2013; Wei et al., 2014). Li et al. (2015) tested pure pentanol in a conventional diesel engine and achieved the ultralow NO_X and smoke emissions without exhaust gas recirculation (EGR), demonstrating its good potential applicability.

Fundamental combustion research can help the clean and efficient utilization of alcohols. Up to now, extensive studies concentrated on the low alcohols. Konnov et al. (2011) and Bradley et al. (2009) respectively studied the laminar combustion characteristics of ethanol with heat flux method and spherically propagating flame. Gu et al. (2010), Veloo and Egolfopoulos (2011) and Wu and Law (2013) subsequently measured the laminar flame speeds of butanol isomers using different apparatuses at the initial pressures of 0.1—0.75 MPa. Cancino et al. (2011) measured the ignition delay times of ethanol-containing gasoline surrogates in a shock tube at

the temperatures from 720 to 1220 K. Moss et al. (2008) and Stranic et al. (2012) studied the auto-ignition characteristics of butanol isomers at the elevated temperatures and the pressures of 1.5–43 atm. Fundamental researches on high alcohol of pentanol fuels started in the latest years. Li et al. (2013a,b) comparatively studied the laminar combustion and chemical kinetic characteristics of 1-, 2-, and 3-pentanol, and reported that 1-pentanol gives the highest flame speed, followed by 3-pentanol and 2-pentanol. Tang et al. (2013) studied the ignition delay characteristics of 1-pentanol, iso-pentanol and 2-methyl-1-butanol using a shock tube, indicating 1-pentanol has the shortest ignition delay. These studies provided valuable insight into the difference among the isomers.

Alcohols are flammable fuels and the alcohol vapors might burn or explode, leading to disasters. Such accidents could happen in the case of fuel evaporation or leakage especially under a high temperature, resulting in properties losses and even human casualties (Dorofeev et al., 1995; Wang et al., 2014a,b). Therefore, the safety issue claims high concern over the fuel utilization, storage and transportation, calling for the demand of investigation on the explosion characteristics to assess the potential explosion hazard. In the previous studies, the main attention was focused on the gaseous fuels like methane, natural gas and ethylene, etc. (Dahoe, 2005; Razus et al., 2007, 2011; Tang et al., 2009, 2014; Zhu et al., 2012; Movileanu et al., 2013; Wang et al., 2014a,b). Their studies demonstrated that the explosion parameters are strongly dependent on initial pressure, initial temperature and fuel/air ratios. Until now, limited researches have been performed on the explosion properties of alcohols. Chang et al. (2009) determined the critical explosion properties of the toluene–methanol mixtures at varied blending ratios and initial oxygen concentrations using a closed spherical vessel, and provided a triangular flammability diagram for the explosive hazard region. Cammarota et al. (2012) studied the explosion characteristics of pure ethanol and ethanol–hydrogen–air mixtures at different equivalence ratios and temperatures using a cylindrical chamber. Zhang et al. (2009) studied the explosion characteristics of methanol–air–diluent mixtures in a constant chamber, from evaluating the peak combustion pressure, flame development duration and combustion duration. Shimy (1970) proposed the formulas for the prediction of the ignition temperature and flammability of alcohols and hydrocarbons. To our knowledge, no report was published for the influence of structures and carbon chain length on the explosion characteristics of alcohols.

In this study, the explosion characteristics of 1-, 2-, and 3-pentanol–air mixtures were studied at initial temperatures from 393 to 433 K and initial pressures from 0.1 to 0.75 MPa using a constant combustion vessel. Explosion hazard was assessed by the explosion parameters such as explosion pressure, deflagration index, maximum rate of pressure rise, combustion duration. The discrepancies among the isomers were analyzed and the effects of the initial conditions on the explosion characteristics were discussed. Meanwhile, a comparative assessment on the explosion characteristics of ethanol-, 1-butanol- and 1-pentanol–air mixtures at different equivalence ratios was also made to evaluate the influence of carbon chain length on the potential risk and hazard of these primary alcohols.

2. Experimental setup and data acquisition

Fig. 1 gives the sketch of the experimental setup. It is composed of ignition system, heating system, constant volume vessel, data acquisition system and inlet/exhaust system. The constant volume vessel is a stainless cylinder with a diameter of 180 mm and length of 210 mm. The mixture in the vessel is ignited by the centrally located electrodes with the spark produced by a standard capacitive discharge ignition system. The spark energy is 45 mJ which is higher than the minimum ignition energy of all the mixtures involved in present study. Heating tapes are wrapped around the chamber to heat the chamber. The temperature in the chamber is monitored by a thermocouple with an accuracy of ± 1 K. The combustion pressure is acquired with a pressure transducer (Kistler 7001) at a sample-rate of 100 kHz connected with a Charge Amplifier (Kistler 5011), and the pressure data was recorded with an oscilloscope. Other control components such as the intake and outlet valves are all mounted on the chamber.

When the chamber was heated to the target temperature, the chamber was vacuumed and repeatedly flushed with dry air to remove the residual gases from the previous experiment. The
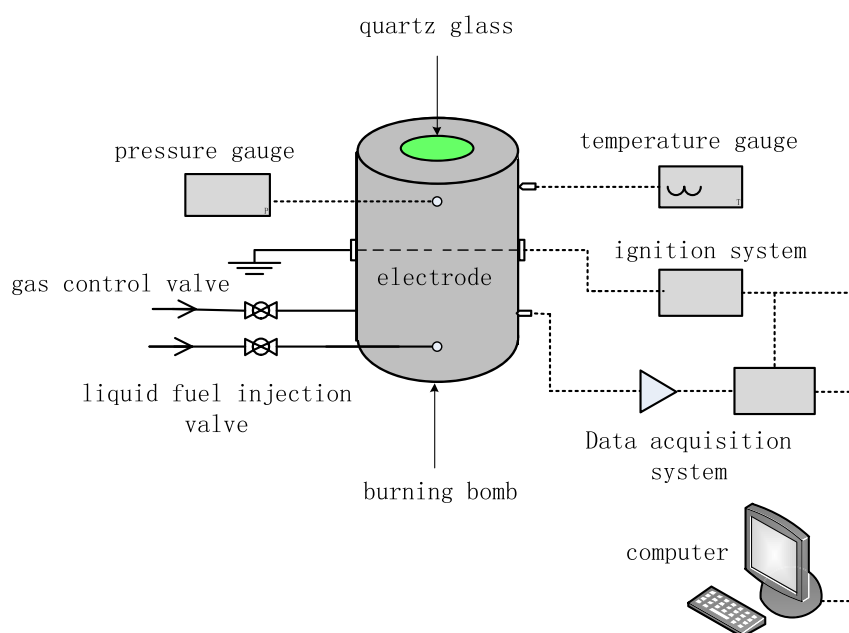

Fig. 1. Experimental setup.