Fuel 211 (2018) 95–101

Contents lists available at ScienceDirect

Fuel

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

Full Length Article

Experimental and kinetic studies of premixed laminar flame of acetone-butanol-ethanol (ABE)/air

Zunhua Zhang[a,b], Shihao Zhu[b], Junjie Liang[b], Le Tian[b], Gesheng Li[a,b,*]

[a] *Key Laboratory of High Performance Ship Technology (Wuhan University of Technology), Ministry of Education, Wuhan, Hubei 430063, PR China*
[b] *School of Energy and Power Engineering, Wuhan University of Technology, Wuhan, Hubei 430063, PR China*

ARTICLE INFO

Keywords:
Acetone-butanol-ethanol
Laminar burning velocity
Outwardly expanding spherical flame
Chemical kinetic analysis

ABSTRACT

In the present study, the experimental study on the laminar burning velocities and Markstein lengths of ABE mixtures and its components was performed in a constant-volume combustion vessel. In addition, a detailed mechanism was employed to simulate the one-dimensional (1-D) premixed laminar flames of ABE mixtures and its components. Results show that the laminar burning velocities of ABE mixtures are slower than those of ethanol, faster than those of acetone, and close to those of *n*-butanol. Moreover, the Markstein lengths of ABE mixtures are close to those of *n*-butanol, indicating that the instability of laminar flames of ABE mixtures is also similar to that of *n*-butanol. The results of kinetic analysis show that the consumption channels of acetone, ethanol and *n*-butanol in single component fuel/air flame and ABE/air flame are very close, respectively. In addition, ABE mixtures and *n*-butanol share a great similarity for the results of sensitivity analysis.

1. Introduction

The decreasing fossil fuel reserves and increasing environmental pollution problems have encouraged researchers to focus on alternative fuels. *N*-Butanol also called bio-butanol [1] is widely considered as a kind of excellent alternative fuel because it has high energy density, low volatility, low moisture absorption and low corrosive properties [2–6]. *N*-Butanol is mainly produced by acetone-butanol-ethanol (ABE) fermentation [7,8]. However, extra energy is required to extract bio-butanol during the ABE fermentation process, which increases the costs of the production of bio-butanol and constrains the application of bio-butanol in engines [9–11].

ABE mixtures are the intermediate product in the ABE fermentation process and the typical volume percentage of acetone, *n*-butanol and ethanol are at 30%, 60% and 10% (A:B:E = 3:6:1 in liquid volume) respectively in industrial production [12]. Recently, some studies showed that ABE mixtures could be used directly in Internal Combustion (IC) engines. Chang et al. [13] studied the water-containing ABE diesel blends fueled in a diesel engine and found that a diesel emulsion with 20 vol% ABE-solution and 0.5 vol% water (ABE20W0.5) enhanced the brake thermal efficiencies and reduced the emissions of particulate matter (PM), nitrogen oxides (NOx), polycyclic aromatic hydrocarbons (PAHs) compared to regular diesel. Zhou et al. [14] studied the combustion characteristics of ABE and diesel blends in a constant-volume combustion vessel under both conventional diesel combustion and low temperature (LTC) conditions. The results demonstrated that 20 vol% ABE (ABE20) mixed with diesel had better combustion efficiency compare to pure diesel. Wu et al. [12] studied the combustion characteristics of the 20 vol% ABE fuels with different component ratio (A:B:E of 6:3:1; 3:6:1; 0:10:0) and mixed with 80 vol% diesel. The results showed that the combustion characteristics of ABE20 (6:3:1) are similar to those of pure diesel. These studies indicate that ABE mixtures are the potential alternative fuels for IC engines.

The parameters of the premixed laminar combustion characteristics such as laminar burning velocities are important because they can comprehensively embody the reactivity, diffusion and heat release in combustion process of fuels, and are the basic parameters of the simulation of turbulent flames and in-cylinder combustion of engines. In addition, the laminar burning velocities are the relevant safety parameters and helpful for the safe industrial use of liquid fuels [15,16]. Also, the parameters of premixed laminar characteristics are also important for the validation of the chemical kinetic mechanisms. Currently the premixed laminar combustion characteristics of acetone, *n*-butanol and ethanol have been studied extensively. Bradley et al. [17] studied the laminar combustion characteristics of ethanol/air laminar flame at 1.4 MPa. Liao et al. [18] studied the effects of initial temperatures on laminar flames of ethanol. Gu et al. [19] studied the effect of initial pressures on the premixed laminar flame of butanol. Gu et al. [20] studied the laminar burning characteristics of diluted *n*-butanol/air mixtures. Broustail et al. [21] carried out the determination of

---

[*] Corresponding author at: Key Laboratory of High Performance Ship Technology (Wuhan University of Technology), Ministry of Education, Wuhan, Hubei 430063, PR China.
E-mail address: gsliwh@gmail.com (G. Li).

http://dx.doi.org/10.1016/j.fuel.2017.09.063
Received 25 June 2017; Received in revised form 13 September 2017; Accepted 15 September 2017

laminar burning velocities for butanol/*iso*-octane and ethanol/*iso*-octane blends for different initial pressures. Nilsson et al. [22] carried out experimental and modeling studies of laminar burning velocities of acetone in air at room and elevated temperatures. However, from the open literatures, the studies of the laminar burning characteristics of ABE/air mixtures are insufficient. Just Van Geem et al. [23] studied the pyrolysis and combustion of ABE mixtures. Hence, to deal with this deficiency, the present study was carried out to experimentally determinate the laminar burning velocities and Markstein lengths of ABE mixtures and its components in a constant-volume combustion vessel at initial temperatures of 358 K, 393 K and 428 K, initial pressures of 0.1 MPa, 0.2 MPa and 0.4 MPa, and equivalence ratios ranging from 0.7 to 1.5 with the interval of 0.1. In addition, a detailed mechanism [24] was employed to perform the chemical kinetic analysis of 1-D premixed laminar flames of ABE mixtures and its components by using CHEMKIN software.

2. Experimental methodologies

2.1. Experimental setup

In the present study, outwardly expanding spherical flames were employed to experimentally investigate the premixed laminar combustion characteristics of ABE mixtures. The detailed validation of the experimental setup has been showed in ref [25]. The related experimental error analysis can be referred to Refs. [25–27]. Only a brief description is presented here.

The schematic of the experimental setup is shown in Fig. 1. The experimental setup mainly consists of a constant-volume combustion vessel, a schlieren optical system, a heating system, an electrical spark generator and a system for data acquisition. The constant-volume combustion vessel was made of stainless steel. The inner diameter and volume of the vessel were 174 mm and 5.86 L, respectively. The two sides of the vessel were mounted with a quartz optical window of 80 mm diameter, respectively. The center of the combustion vessel was mounted with two electrodes of 1.5 mm diameter. The high-speed digital camera operated at the capture of 10,000 frames per second in this study.

At the start of the experiment, the initial temperatures inside the combustion vessel were stabilized at the desired values via the heating system. Then the combustion vessel and piping system were vacuumed by a vacuum pump. After that, the ABE mixtures were injected into the vessel. Then the injected ABE mixtures started to vaporize, and the pressure inside the combustion vessel began to increase. When the reading of the pressure transmitter did not change, air was introduced into combustion vessel according to their respective partial pressures. After standing 10 to 15 min, the ABE/air mixtures in the combustion vessel were homogenous.

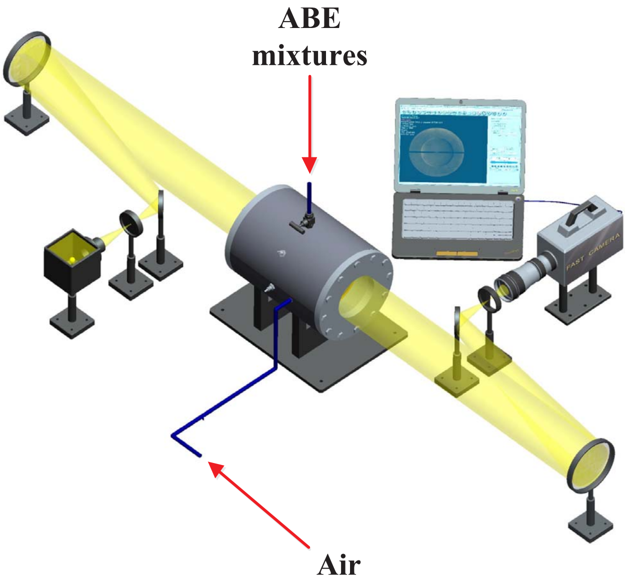

Fig. 1. Schematic of the experimental setup.

In the present study, each experiment was repeated at least three times under the same conditions and the repeatability was good. The standard deviation with 95% confidence interval of the experimental data is used as the uncertainty to present the repeatability of the experiment. The laminar burning velocity determined in the present study has an absolute error of 3 cm/s (the biggest standard deviation with 95% confidence interval of laminar burning velocities) and relative error of 5% (the maximum ratio of standard deviation with 95% confidence interval of laminar burning velocities to the average values of laminar burning velocities) approximately. It should be noted that, the error bar given in the figures presenting the experimental data just reflects the repeatability of the experimental data. As demonstrated in the recent study, the uncertainty in equivalence ratio can greatly affect the accuracy of laminar burning velocity measurement using propagating spherical flames [28]. So the uncertainty of equivalence ratio is calculated and available in Supplemental Material.

In addition, the typical liquid volume percentage of acetone, *n*-butanol and ethanol are at 30%, 60% and 10% (A:B:E = 3:6:1) respectively in ABE mixtures. The purities of acetone, *n*-butanol and ethanol were respective 99.5%, 99.5% and 99.8% and the air was a mixture of 21% oxygen and 79% nitrogen in volume.

2.2. Data processing

For outwardly expanding spherical flame, the stretched flame speed S_n can be computed according to *R*-*t* by

$$S_n = \frac{dR}{dt} \tag{1}$$

where *R* is radius of flames, *t* represents time.

For spherical flames, the stretch rate α is the relative rate of the change of the flame surface area i.e. [29]

$$\alpha \equiv \frac{1}{A}\frac{dA}{dt} = \frac{2}{R}\frac{dR}{dt} = \frac{2}{R}S_n \tag{2}$$

where *A* is the flame surface area in flame front.

The unstretched flame speed, S_l, is derived from the relationships between S_n and α. They are [30–32]

$$S_l - S_n = L_b\alpha \tag{3}$$

and

$$\left(\frac{S_n}{S_l}\right)^2 \ln\left(\frac{S_n}{S_l}\right)^2 = -\frac{2L_b\alpha}{S_l} \tag{4}$$

where L_b is the Markstein length, which reflects the instability of flames.

The results, especially the Markstein length, are strongly affected by the linear or nonlinear model used in data processing [33,34]. Fig. 2 shows the variations of the stretched flame propagation speed for ABE/air mixtures against the stretch ratio at 393 K and 0.1 MPa. It can be observed that the nonlinear fitting is consistent with experimental values better than the linear fitting. Hence, in the present study nonlinear fitting was used to process experimental data.

In addition, recent studies have suggested to directly compare the measured quantities instead of extrapolated ones with 1-D simulation results predicted by kinetics so that the uncertainty associated with extrapolation can be eliminated. [28] Hence, the data used for linear or nonlinear extrapolation (stretched flame speed as a function of stretch rate) for all different cases (different equivalence ratios, different pressure and different temperatures) are provided in the Supplementary