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Investigation on laminar burning velocities of benzene, toluene and ethylbenzene up to 20 atm

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ABSTRACT

The laminar flame propagation of benzene, toluene and ethylbenzene was investigated at $T_u = 423$ K, $P_u = 1$–20 atm and various equivalence ratios in a high-pressure constant-volume cylindrical combustion vessel. The laminar burning velocities (LBVs) were observed to increase in the order of toluene, ethylbenzene and benzene at both atmospheric and high pressures, and the Markstein lengths were evaluated to be similar among the three aromatic fuels. Three recently developed kinetic models of aromatic fuels were used to simulate the experimental data. Sensitivity analysis was performed to investigate the kinetic effects on LBVs of the three aromatic fuels under various conditions. Different from the cases of alkane LBVs, the reactions of fuel-specific species are important for the LBVs of the three aromatic fuels at 1–20 atm, especially for the LBVs under rich conditions. In particular, the pyrolysis reactions in the sub-mechanism of aromatic fuels play a dominant role in negatively sensitive reactions under rich conditions, indicating prominent inhibition effects of aromatic flame chemistry on the LBVs. The sensitivity variation analysis and normalized sensitivity variation analysis indicate that the importance of most of the small species and fuel-specific species reactions are enhanced with increasing pressure, especially under rich conditions. The pressure effects of the flame chemistry on the aromatic LBVs strongly depend on the reaction circumstance. A series of chain termination reactions and chain propagation reactions producing less active radicals have large negative sensitivity coefficients and are generally more susceptible to the pressure variation than the positively sensitive reactions. The modeling analysis indicates that aromatic flame chemistry inevitably changes to resist the enhanced combustion intensity with increasing pressure.

1. Introduction

Laminar burning velocity (LBV) is one of the most important combustion parameters. It is not only useful for understanding the exothermicity, diffusivity and reactivity in combustion, but also strongly involved in the determination of turbulent burning velocity [1,2]. In particular, investigations on the LBVs of transportation fuels and their components with relatively high boiling points (BPs, refer to 1 atm value in this work) are of special importance for engine combustion research, especially at engine-relevant pressures which are usually higher than 10 atm [3], since engines are generally operated at high pressures to reach higher efficiency and power output. The increase of pressure greatly enhances the molecular collision in flame and significantly changes reactivity [2], leading to great differences between high pressure combustion and atmospheric pressure combustion.

Aromatic hydrocarbons are critical components in transportation fuels, such as gasoline, jet fuels and diesel oils, as well as their surrogate fuels [4–8]. The properties and combustion characteristics of aromatic fuels are different from those of alkanes due to the existence of benzene ring and consequently stable molecular structures [2,9–11]. Among aromatic fuels, benzene, toluene and ethylbenzene are representative ones and of special interest because of their substantial fractions in transportation fuels and surrogate fuels [4–8]. A number of investigations have been performed on the LBVs of benzene, toluene and ethylbenzene [7,11–25], mainly at atmospheric pressure [7,12–14,16–21,23,24]. Counterflow flame was the most frequently used method to determine the LBVs of benzene and toluene [12–14,16–19,21,22]. Ji et al. [18] measured the LBVs of monocyclic aromatic fuels with one or several side alkyl chains at 1 atm and concluded that increased methylation in aromatic fuels results in reduced LBVs. Hui et al. [19] found that *n*-propylbenzene has the highest reactivity followed by toluene and trimethylbenzenes at 1 atm. In addition, several studies have adopted heat flux method to measure the LBVs of the three aromatic fuels at atmospheric pressure [7,20,23]. The LBVs of

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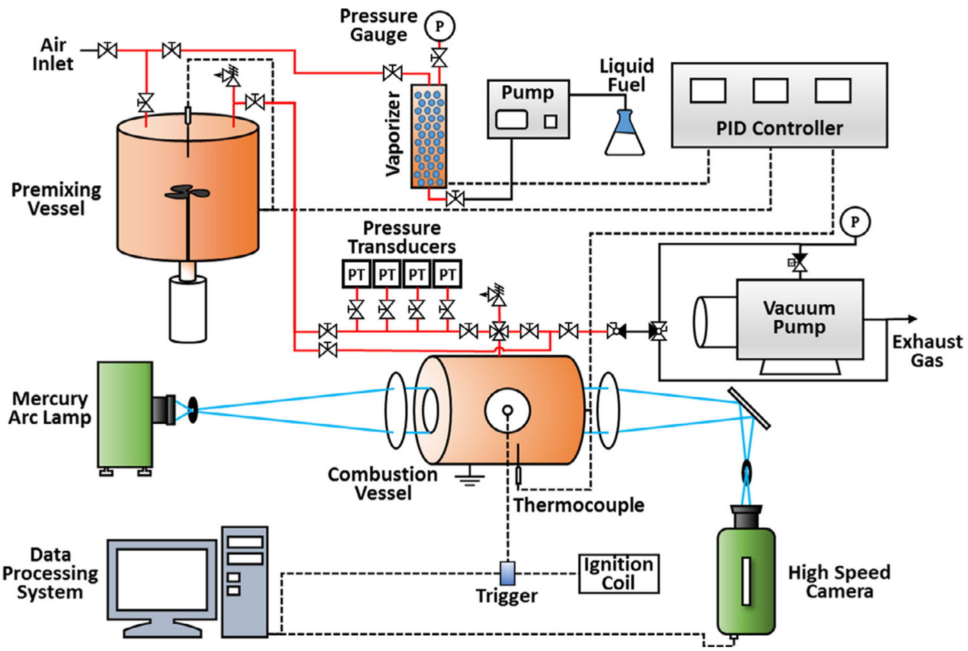

Fig. 1. Schematic diagram of the constant-volume single-chamber cylindrical combustion vessel apparatus. The heated pipezzlines and vessels are denoted with red color and orange color, respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

ethylbenzene, *n*-propylbenzene and *n*-butylbenzene were measured by Mehl et al. [7] and the results showed that a higher propensity to form benzyl radical results in a lower LBV. Most recently, Meng et al. [24] studied the LBVs of styrene and ethylbenzene using spherically expanding flame and confirmed that the different concentrations of benzyl radical causes their different LBVs.

To the best of our knowledge, only few studies of aromatic LBVs have been performed at pressures higher than 1 atm [15,22,25]. Johnson and Farrell [15] measured the LBVs of benzene, toluene and ethylbenzene using spherically expanding flame at the initial pressure (P_u) of 3 atm, unburnt temperature (T_u) of 450 K and equivalence ratios (ϕ) of 0.8–1.4. Hui et al. [22] built a high-pressure counterflow flame apparatus and used it to measure the LBVs of toluene at $P_u = 1–3$ atm. Most recently, Han et al. [25] measured the LBVs of toluene at $P_u = 1–5$ atm and *o*-xylene at $P_u = 1–2$ atm using a dual-chamber vessel. Fuel chemistry was considered as the primary reason for the faster propagation of the toluene flame than that of the *o*-xylene flame in [25]. In general, reaction kinetics is found to be a critical factor for aromatic LBVs which strongly depend on the molecular structure of aromatic fuels [18]. Nevertheless, kinetic effects on aromatic LBVs has only been studied within a narrow pressure range, and mainly for stoichiometric flames [7,18,19,25].

It is also realized that the highest investigated P_u (5 atm) for the LBVs of aromatic fuels is much lower than the engine-relevant pressures. This reveals the challenge in LBV measurements of liquid fuels at engine-relevant pressures, especially for those with BPs higher than 373 K. In a recent survey from nearly 120 papers published in major combustion journals on the experimental determination of LBVs of different kinds of fuels, Xiouris et al. [26] concluded that only 27% studies were performed at high pressures. Moreover, the number of studies for gaseous fuels is notably larger than that for liquid fuels among the high-pressure measurements. Consequently, the measurements of high-pressure LBVs of liquid fuels, especially the high BP fuels, are desired for the understanding of their laminar flame characteristics, validation of kinetic models and real engine researches.

This work aims to measure the LBVs of benzene, toluene and ethylbenzene at P_u up to 20 atm. The BPs of the three fuels are 353.3 ± 0.1, 383.8 ± 0.2 and 409.3 ± 0.3 K [27]. Combustion vessel has many advantages for the measurements of LBVs at high pressures [28]. In particular, single-chamber combustion vessel is feasible for external heating at high temperatures and has the potential to satisfy the research demand for high BP fuels. A constant-volume single-chamber cylindrical combustion vessel has been built for this target and is introduced in detail in this work. The second target is to investigate the influence of high pressure on the LBVs of aromatic fuels based on both experimental observations and modeling analysis. Three recently developed kinetic models of aromatic fuels were applied and their performances were examined over wide pressure and equivalence ratio ranges. Sensitivity analysis, sensitivity variation analysis and normalized sensitivity variation analysis were performed to provide insight into the flame chemistry at different pressures and equivalence ratios. Special attentions were paid on the kinetic effects and pressure effects on LBVs.

2. Experimental method

Figure 1 shows the schematic diagram of the experimental apparatus. The combustion vessel is made of 304 stainless steel and has an inner volume of 2.77 L (inner diameter 150 mm, inner length 152 mm). The asymmetry effect of non-spherical vessel can be largely weakened by applying near-unity length-diameter ratio [28,29]. The vessel was hydrostatically tested to 200 atm. Two quartz windows (diameter 100 mm, thickness 30 mm) were clamped to the vessel flange, providing an optical access with 75 mm diameter clear apertures.

Partial pressure method was used for preparing combustible mixtures in the premixing vessel. Xiouris et al. [26] concluded that the uncertainty in the pressure indication is a certain percentage of the full range of the device. Thus, four pressure transducers with different full ranges including 0.1, 0.5, 2.0 and 8.0 MPa were used in order to improve the accuracy. All vessels and pipelines were evacuated to about 20 mTorr before charging. The liquid fuels were vaporized in an electrically heated vaporizer before the injection to the premixing vessel. The prepared mixtures were stirred by a magnetic stirrer for 10 min to ensure uniform mixing. The