



## Full Length Article

# Experimental and kinetic study on laminar flame speeds of styrene and ethylbenzene



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## HIGHLIGHTS

- Laminar flame speeds of styrene and ethylbenzene were measured.
- Three chemical kinetic models of styrene and ethylbenzene were validated.
- The chemical kinetic analysis of styrene and ethylbenzene were performed.

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## ABSTRACT

An experimental and numerical study was performed on laminar flame speeds of styrene and ethylbenzene at the equivalence ratios of 0.8–1.5, initial temperatures of 358 K, 398 K and 450 K and atmospheric pressure in a heated cylindrical constant volume chamber with volume of 5.58 L. The experimental results revealed that styrene has the faster laminar flame speeds and the larger Markstein lengths than ethylbenzene. Three chemical kinetic models (Narayanaswamy model, Yuan model and NUI model) were tested against the present experimental data, and the results calculated by Yuan model showed the best agreement. Furthermore, the chemical kinetic analysis was conducted. The sensitivity analysis revealed that the benzyl radical has negative effect on laminar flame speeds and is responsible for the differences in the laminar flame speeds between styrene and ethylbenzene. The reaction pathways analysis showed that the different branching ratios of fuel molecular decomposing to benzyl cause the discrepancies in the concentration of benzyl radical in styrene and ethylbenzene flame. It can be concluded that the higher benzyl radical concentration results in the slower laminar flame speed.

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## 1. Introduction

Aromatics are the key components of practical engine fuels such as gasoline, diesel and jet fuel [1,2]. The addition of aromatics can enhance the energy density of fuels, increase octane ratings of fuels which can result in improving antiknock performance and easily form soot during the engine combustion. Furthermore, the existence of aromatics in transportation fuels has significant influence on combustion characteristic, such as laminar flame speed, extinction limit, ignition delay time and tendency of soot formation [3,4]. Fundamental combustion research on aromatics are useful to establish accurate surrogate model of practical fuels and can provide the mechanism of soot formation in engine. Hence, it is necessary to study the combustion characteristics of aromatics. The

laminar flame speed is an important parameter for combustor design and also used to validate chemical kinetic models.

Some researchers have studied on the combustion characteristics of alkyl-benzene in literatures. Ji et al. [5] measured extinction strain rates and laminar flame speeds of toluene, o-, m- and p-xylene, and 1,2,4- and 1,3,5-trimethylbenzene by using the counterflow setup at initial temperature of 353 K and pressure of 0.1 MPa. The results showed that the laminar flame speeds decreased with the increased methylation on the benzene ring, as follows: toluene > xylene > trimethylbenzene. Mehl et al. [6] systematically measured the laminar flame speeds of alkylbenzene from the toluene to heavier butylbenzene at different initial gas temperatures (358 K and 398 K) and atmospheric pressure in a premixed flat-flame burner using the heat flux method. The results showed the laminar flame speeds of alkylbenzene-air mixtures were decreased in the order of ethylbenzene > propylbenzene ≥ butylbenzene > toluene. Johnston and Farrell [7] studied the laminar flame speeds and Markstein lengths of benzene,

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toluene, ethylbenzene, m-xylene and n-propyl-benzene with equivalence ratios from 0.8 to 1.4 at temperature of 450 K and pressure of 304 kPa. The laminar flame speeds were consistent with the results reported by Mehl et al. While the results showed that the benzene has the largest Markstein lengths, followed by m-xylene, toluene and ethyl- and propyl-benzene. Li et al. [8] measured species in three premixed ethylbenzene/O<sub>2</sub>/Ar flames with equivalence ratio of 0.75, 1.0 and 1.79, at pressure of 4.0 kPa using synchrotron vacuum ultraviolet photoionization mass spectrometry. The experimental results were used to validate a kinetic model of ethylbenzene and revealed the decomposition of ethylbenzene and the formation of PAHs. Furthermore, Li et al. [9] investigated rich premixed ethylbenzene flame at 4.0 kPa pressure using molecular-beam mass spectrometry (MBMS) and tunable synchrotron vacuum ultraviolet (VUV) photoionization. The results showed that the formation of typical PAHs can be related to the H-abstraction/C<sub>2</sub>H<sub>2</sub>-addition mechanism.

Although some fundamental combustion research on the alkylbenzene, there is limited research focused on alkenyl-benzene. In most aromatic flames, styrene is an important intermediate and can be produced not only from the pyrolysis of aromatic fuels but also through the reactions of cyclopentadienyl radical with propargyl radical and 1,3-cyclopentadiene [10]. Especially in rich aromatic flames, the high concentration of styrene are important and can be also measured [11]. So, styrene is a key precursor of the polycyclic aromatic hydrocarbons (PAHs) [12]. Moreover, styrene is an important petrochemicals to produce various types of copolymers that are the materials to form plastics and synthetic rubbers [13]. Therefore, the combustion characteristics of styrene combustion is necessary to be thoroughly investigated.

Pengloan et al. [14] measured the ignition delay times of styrene in a shock-tube over the temperature ranges from 1300 K to 2000 K and the pressure of 1.43 atm. Grela et al. [15] employed on-line mass spectrometry to investigate the decomposition of styrene at temperatures of 1180–1350 K in a low-pressure flow reactor. The results showed that benzene and vinylidene are the intermediates of the styrene consumption. Yuan et al. [13] measured the species of styrene/benzene mixtures oxidation in JSR at lean, stoichiometric and rich conditions. A detailed chemical kinetic mechanism of styrene was proposed and validated by the experimental data. There is no laminar flame speeds of styrene in published literatures.

Therefore, one object of this study was to obtain new experimental laminar flame speeds of styrene using a constant volume chamber. Then, ethylbenzene was selected as the comparative fuel considering the analogous molecular structure with styrene. Three different chemical kinetic models for aromatic were employed and the calculated results were compared to the experimental laminar flame speeds. Finally, the reaction pathways analysis was conducted to give the explanations on the differences in laminar flame speeds between styrene and ethylbenzene.

## 2. Experimental setup and data processing

### 2.1. Experimental setup

In this study, the laminar flame speeds were measured using the outwardly spherical propagating flame method. A detailed description of the experimental apparatus has been published elsewhere [16,17], and only a brief introduction is given here. The combustion chamber is cylindrical with volume of 5.58 L, and two pressure-resisting quartz windows with the diameters of 80 mm are located on the two sides for optical access. A 1.5 kW heating-tape is wrapped around the chamber and the temperature is calibrated by an S type thermocouple with an accuracy of 3 K.

The composition of mixtures are introduced into the chamber by a micro-adjustable valve and by a high precision pressure transmitter. To eliminate the effects of incomplete mixing and gas motion, the mixtures are kept at least 3 min in the chamber before ignited by the centrally located electrodes. The propagation of spherically expanding flames are recorded by a high-speed digital camera Phantom V611 at 10,000 frames per second.

Styrene and ethylbenzene used in this experiment were purchased from Energy-Chemical Limited Co., with purity of  $\geq 99\%$  and  $\geq 99.5\%$  respectively. Because of the low vapor pressure of the two test fuels, the ranges of equivalence ratio were set from 0.8 to 1.5 at initial pressure of 0.1 MPa and temperatures of 398 K and 450 K. To compare with the data from literature, the laminar flame speeds of ethylbenzene were measured at 358 K and 0.1 MPa pressure additionally.

### 2.2. Extraction of the laminar flame speed

For a stable outwardly spherical propagating flame, the stretched flame propagation speed can be calculated according to  $S_b = dr/dt$ , where  $r$  is the flame radius. The non-linear extrapolation method proposed by Kelly and Law [18] was applied to calculate the unstretched flame propagation speed  $S_b^0$ , and the formula is expressed as:

$$\left(\frac{S_b}{S_b^0}\right)^2 \ln\left(\frac{S_b}{S_b^0}\right) = -2\frac{L_b k}{S_b^0} \quad (1)$$

where  $L_b$  is the Markstein length. The flame stretch rate,  $k$ , is represented as

$$k = \frac{1}{A} \frac{dA}{dt} = 2S_b/r \quad (2)$$

Besides nonlinear extrapolation method, the linear extrapolation method was also discussed in this study, and the equation is expressed as:

$$S_b = S_b^0 - L_b k \quad (3)$$

Finally, the laminar flame speed,  $S_u^0$ , can be determined through

$$S_u^0 = S_b^0 \rho_b / \rho_u \quad (4)$$

where the  $\rho_b$  and  $\rho_u$  are the burned and unburned gas densities, respectively.

### 2.3. Experimental uncertainty analysis

High-quality measurement of laminar flame speed are affected by various factors including flame instability [19,20], ignition [21,22], chamber confinement [23–25], buoyancy [26], radiation [27,28], extrapolation method [29] and mixture preparation [30]. To minimize the effects of ignition energy and chamber confinement, the flame radius range of 8–24 mm was adopted in the  $S_b^0$  extraction. In addition, the flame photos with cellular structures was neglected during the data processing.

Radiation is another factor which can affect the flame propagation speed via radiation heat loss and radiation reabsorption [31]. The effect of radiation heat loss can reduced the flame propagation speed while the flame propagation speed can be accelerated by radiation reabsorption. So, the radiation effect should be evaluated according to the equation of Yu et al. [27], as follows:

$$S_{u,RCFS}^0 = S_{u,Exp}^0 + 0.82 S_{u,Exp}^0 (S_{u,Exp}^0/S_0)^{-1.14} (T_u/T_0)(P_u/P_0)^{-0.3} \quad (5)$$

where  $T_0 = 298$  K,  $S_0 = 0.01$  m s<sup>-1</sup>,  $P_0 = 0.1$  MPa;  $S_{u,RCFS}^0$  and  $S_{u,Exp}^0$  are radiation-corrected laminar flame speed and measured laminar flame speed, respectively.

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