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Laminar burning velocities of benzene + air flames at room and elevated temperatures

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HIGHLIGHTS

- The burning velocities of benzene + air flames at several temperatures were measured.
- Comparison of predictions of 3 mechanisms with the experimental data showed mixed agreement.
- The temperature dependence of the burning velocity was interpreted using an empirical power law.
- Detailed model from Politecnico di Milano performs the best over the range of conditions studied.

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ABSTRACT

Laminar burning velocities, S_L, of benzene + air flames were determined at atmospheric pressure and initial gas temperatures, T, of 298, 318, 338 and 358 K. Non-stretched flames were stabilized on a perforated plate burner using the heat flux method. New measurements were compared with available literature results obtained in spherical and counterflow flames at room and elevated temperatures. Data consistency was assessed with the help of analysis of the temperature dependence of the laminar burning velocity, which was interpreted using an empirical expression $S_L = S_{L0}(T/T_0)^{\alpha}$. Both the laminar burning velocities and the power exponents, α, were compared with predictions of three kinetic mechanisms: JetSurF 2.0, and two models for kerosene developed at Politecnico di Milano: Skeletal Surrogate (121 species) and high-temperature detailed (ver. 1412). The last model demonstrated the best performance over the range of conditions studied.

1. Introduction

Aromatic hydrocarbons are present in all conventional liquid transportation fuels, such as gasoline [1], diesel [2,3] or jet fuels (kerosene) [4]. Because of the complexity of real fuels, containing hundreds components often of varying composition, fuel surrogates consisting of a few class-representative hydrocarbons are used in laboratory experiments and in combustion modelling [5]. Development and validation of kinetic models for surrogate fuels capable in predicting different combustion phenomena, therefore, require accurate knowledge of pertinent characteristics of individual components, such as ignition delays or burning velocities.

Combustion chemistry of benzene, the simplest aromatic hydrocarbon, has been studied in jet-stirred and flow reactors, in shock tubes and in flames, as summarised recently by Saggese et al. [6]. Detailed kinetic model of benzene combustion developed at Politecnico di Milano [6] demonstrated overall good performance in a wide range of conditions from pyrolysis to very lean oxidation. The laminar burning velocity, important characteristic of benzene + air mixtures, which depends only on stoichiometric ratio, ϕ, temperature and pressure, was calculated as well and compared with experimental data of Davis and Law [7], of Johnston and Farrell [8] and of Ji et al. [9]. Good agreement was found with the measurements at standard conditions (1 atm and initial mixture temperature of 298 K) [7], and at elevated pressure of 3 atm and initial temperature of 450 K [8]; however, most recent measurements at 1 atm and initial temperature of 353 K [9] significantly diverge from the model predictions. This comparison indicates that experimental datasets obtained at different temperatures might be inconsistent. The inconsistency was also observed by Ji et al. [9], who scaled original data of Davis and Law [7] to higher temperature of 353 K using ratio of the burning velocities predicted by kinetic modelling.

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Various factors may affect reliability of the experimental data and contribute to uncertainties of the burning velocity measurements depending on the experimental method and data processing as reviewed by Egolfopoulos et al. [10]. All available studies of the burning velocity, S_L, of benzene + air mixtures are summarised in Table 1. Davis et al. [11] investigated counterflow flames at standard conditions and derived burning velocities using linear and non-linear stretch corrections. Non-linearly extrapolated S_L were found, on average, about 2 cm/s lower than the linearly extrapolated values. Davis and Law [7] revisited benzene + air flames in a wider range of equivalence ratios due to improvements in flame stability and stated that their linearly extrapolated data did not change much from those previously reported [11]. Wang et al. [12] used linear stretch correction and examined various counterflow configurations: twin flames, premixed flame against nitrogen counterflow or against air counterflow. Different counterflow configurations yielded largely different (by 3–4 cm/s at 363 K) burning velocities, and even different values for upper and lower twin flames; this dataset is therefore usually ignored in the validation of kinetic models. Farrell et al. [13] performed extensive comparative study of molecular structure effects on S_L for 45 hydrocarbons; no stretch correction was considered since the burning velocities were derived from pressure – time traces. Johnston and Farrell [8] at the same elevated temperature and pressure processed Schlieren images and obtained S_L using linear stretch correction. The burning velocities derived without [13] or with stretch correction [8] significantly differ both in maximum values and in the shape of the S_L dependence on equivalence ratio. Ji et al. [9] implemented counterflow technique similar to the earlier studies [7,11,12], yet applied computationally assisted non-linear extrapolation to zero stretch, which is currently considered to be an advanced approach for the counterflow data processing [10].

In the view of different S_L derived using linear or non-linear stretch correction and inconsistency between experimental datasets obtained at different temperatures mentioned above, the measurements of the burning velocity of non-stretched flat flames generated by the heat flux method at different initial temperatures could be most helpful, and this was the primary goal of the present study. In addition, the paper presents a comparison of the experimental results with the modelling using three kinetic mechanisms: JetSurF 2.0 [14], and two models for kerosene developed at Politecnico di Milano: high-temperature detailed (ver. 1412) [15] and Skeletal Surrogate (121 species) [16].

2. Experimental details

The heat flux method was used to determine the laminar burning velocities of premixed benzene + air flames at atmospheric pressure (1005–1015 hPa) and initial gas temperatures of 298, 318, 338 and 358 K. The flames were studied over the equivalence ratio range of 0.6–1.5. No soot formation was observed at all equivalence ratios studied. The benzene was provided by Sigma–Aldrich with the purity better than 99%. Basic principles behind the heat flux method have been described in detail in many previous publications, e.g. [17–25]; the method was also reviewed by Egolfopoulos et al. [10] together with two other contemporary techniques for measuring S_L, namely counterflow flames and spherically expanding flames. Through more than 20 years of the development, several improvements were introduced in the heat flux method as described by Bosschaart and de Goey [17] and recently by Alekseev et al. [18]. In the following, only essential features of the experimental procedure and modified data processing are outlined in relation to the evaluation of experimental uncertainties.

Schematic of the experimental setup employed in the present study was originally depicted in [19] with the latest modifications shown and described by Christensen et al. [20]. Design of the heat flux burner was essentially the same as introduced by Bosschaart and de Goey [17] with cross-section and technical details of the burner head and of the burner plate presented recently in [21,22].

Laminar flames are stabilized above the burner plate via heat loss of the flame to the burner. These heat losses are compensated by heating the burner plate to temperatures above that of the unburned gas, and creating a temperature increase of the unburned gas as it passes the perforated burner plate. The difference in the heat loss and heat gain of the burner plate results in a parabolic temperature distribution that can be measured using thermocouples inserted into several holes of the perforated burner plate. Temperature readings from the thermocouples are fitted to the form [17]:

$$T(r) = T_{r=0} + Cr^2 \qquad (1)$$

In this equation $T_{r=0}$ is the temperature at the centre of the burner plate, C is the parabolic coefficient and r is the radial placement of the thermocouples. A typical procedure of measurements of the burning velocity consists in determination of the parabolic coefficient, C, as a function of unburned gas velocity, V_g. The unburned gas velocity is regulated to velocities slightly above and below the adiabatic state, at which $S_L = V_g$ [17], while measuring the temperature profile of the burner plate. The burning velocity can then be found via interpolation.

In the absence of stretch, flat flames of heavy fuels are prone to instabilities mostly manifested in richer mixtures and at elevated initial gas temperatures. This was considered a technical limitation of the heat flux method [19] that restricts the range of conditions actually accessible in experiments. To overcome this limitation, Vancoillie et al. [25] proposed an extrapolation procedure based on the assumption of locally linear variation of the parabolic coefficient, C, with the gas velocity, V_g. In this procedure the gas velocity is set always below and gradually approaching S_L, until the instability is manifested. The extrapolation procedure was successfully implemented in subsequent studies and further illustrated in detail by Naucler et al. [21].

Most recently Alekseev et al. [22] derived a functional form of the parabolic coefficient, which, in simplified form, can be written as:

$$C = A \cdot V_g \cdot \left[\left(\frac{V_g}{S_L} \right)^{\frac{1}{\alpha - 1}} - 1 \right] \qquad (2)$$

Table 1
Experimental studies of the burning velocity of benzene + air mixtures.

Temperature (K)	Pressure (atm)	Eq. ratio	Method	Extrapolation	Source
298	1	0.8–1.4	Counterflow	Linear and non-linear	Davis et al. [11]
298	1	0.7–1.7	Counterflow	Linear	Davis and Law [7]
363	1	0.7–1.3	Counterflow	Linear	Wang et al. [12]
450	3	0.55–1.3	Spherical	No	Farrell et al. [13]
450	3	0.8–1.4	Spherical	Linear	Johnston and Farrell [8]
353	1	0.7–1.5	Counterflow	Computationally assisted non-linear	Ji et al. [9]