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An improved reaction mechanism for predicting the charged species in ethanol-air flame

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ABSTRACT

To predict the charged species distributions in the ethanol-air flame, an improved reaction mechanism is proposed. The detailed reaction mechanism involving neutral species for the combustion of ethanol is combined with a set of ionic reactions to account for the charged species chemistry. The new chemical-kinetic mechanism consists of 64 species and 423 reactions. Simulation of ethanol-air flame involving charged species is conducted by using the model based on the proposed mechanism. The present model is validated by the experimental results. The ethanol-air flame temperature, neutral and charged species distributions are reasonably predicted by the present model. Although the concentrations of charged species are much lower than that of neutral species, the charged species have an important effect on the flame characteristics, especially under the electric field. Electrons are the main negative charged species and H_3O^+ is the main positive charged species in the ethanol-air flame. The results of pathway analysis and sensitivity analysis show the crucial roles of H_3O^+ and the reactions involving it for the charged species chemistry. When the electric field is applied, the present model has a better performance in predicting the diffusion ethanol-air flame compared with the model without charged species.

1. Introduction

Ethanol is the major bio-derived renewable fuels. It has been widely used in internal combustion engines [1]. Moreover, ethanol has a larger octane number and latent heat of vaporization than gasoline, and thus it will increase the thermal efficiency and reduce carbon emissions [2].

Recently, the electric field assisting combustion has been considered as one of the potential technologies to improve and control the combustion process [3,4]. Due to the existence of charged species in the flame, when an electric field is applied, the electric field will have a significant impact on the flame due to the ionic wind [5,6]. In previous studies, the voltage-current characteristics (VCC) [7,8] and the electric resistance of flame in the electric field [9] have been measured. The results showed that the number density of charged particles was about 10^9–$10^{12}\,cm^{-3}$ [10,11]. The chemi-ionization process has been considered as the dominant source of generation of charged species in hydrocarbon combustion [12]. Therefore, a detailed knowledge of the chemi-ionization process for charged species formation as well as chemical kinetic mechanism is needed for modeling the flame dynamics under electric field and interpreting the characteristics and mechanisms [13].

Many studies have been carried out to study the chemical kinetics of ethanol combustion early [14–17]. A detailed mechanism for high temperature ethanol oxidation was reported by Marinov [18] and this mechanism has been validated by experimental data in shock tubes and burning velocities [19]. Li et al. [20] experimentally studied the ethanol decomposition reactions in a variable pressure flow reactor. They developed the mechanism proposed by Marinov and the rate constants of the molecular decomposition reaction were measured. Leplat et al. [21] measured the chemical species in premixed ethanol flame at low pressure and in a jet-stirred reactor at atmospheric pressure and the experimental results were compared to the detailed mechanism assembled by reviewing the literatures. Aghsaee et al. [22] studied the pyrolysis and oxidation of ethanol mixtures at high temperature in a shock tube. The laminar flame speeds of ethanol in air were measured and it was found that the mechanism developed by Ranzi et al. [23] provides the best agreement with the experimental data at high temperature. The chemical mechanism of ethanol combustion has been developed for different conditions. These mechanisms predict the combustion process involving neutral species of ethanol reasonably well.

However, the mechanisms of ethanol combustion including the formation of charged species are very scarce in the literatures. The prediction of charged species in the flame is needed for some situations, especially under electric field or plasma. Prager et al. [24] calculated the laminar flat methane-oxygen flame using a detailed mechanism

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which considered negative ions and discussed the diffusion processes of the ions. It was found that the negative ions and ion–ion recombination reactions are important in fuel-lean flames. Belhi et al. [25] numerically studied the stability of methane flame under electric field. The negative ions were found to be crucial after comparing the results considering anions and neglecting anions. Recently, Alquaity et al. [26] measured the positive ions in methane flame and found the dominant ions and chemi-ionization. Kim et al. [27] improved the quantitative characterization of ion chemistry for methane oxidation and discussed the key pathways to ion and electron formation in flames. However, few studies considered the chemical reactions involving chemi-ionization process for ethanol flames.

The goal of this study is to develop a chemi-ionization kinetic mechanism for ethanol-air combustion, and thus to predict the flame characteristics more precisely, especially under electric field. Firstly, experimental measurements are conducted to obtain the ion densities and flame structures. Secondly, the reaction mechanism for the ethanol-air combustion involving neutral species is used as the base mechanism, and improved by adding a set of ionic reactions. Then, the calculated results are validated by the experimental data. The ion chemistry and charged species distributions are analyzed. The pathway analysis and sensitivity analysis for the present ethanol combustion mechanism with charged species are carried out. Lastly, this mechanism is employed to predict more precisely the ethanol-air flame under electric field.

2. Experimental measurements

The schematic of experimental setup of ion concentration measurement in diffusion ethanol-air flame is shown in Fig. 1. Ethanol (C_2H_5OH) was used as the fuel used in these experiments. Air around the flame as the oxidizer was entrained from the ambient. The burner is based on the diffusion ethanol-air flame and the basic part of system and experimental method are similar to our previous works [28–31]. A uniform electric field is formed between the two parallel electrodes. A digital camera (Canon EOS 5D Mark III) was employed to visualize the flame images. A thermocouple (S type) was used to measure the flame temperature at top position of the flame.

A single filament Langmuir probe was used to obtain ion density in the flame. The Langmuir probe was biased to −5 V by a sourcemeter (Keithley 2450) before being set into the flame. The Langmuir probe was constructed from a 0.15 mm diameter tungsten wire placed in a 1.2 mm outer diameter ceramic tube as sheath. The active length of tungsten wire protruding from the tube was 5 mm. For cylindrical probe with thick sheath, the equation was provided for calculating the ion density as follow [5].

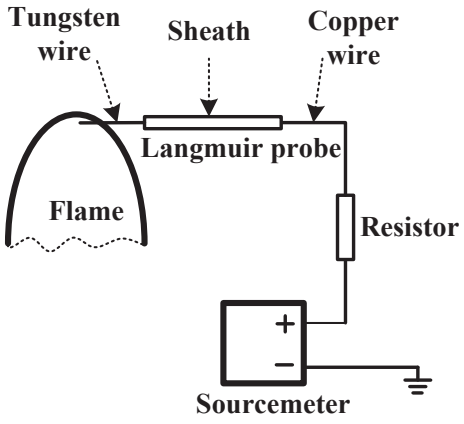

Fig. 1. Schematic of experimental setup of ion concentration measurement.

$$n_i = \left(\frac{I}{5.3(\varepsilon_0 \mu_i)^{0.25} V_b^{0.5} r_p^{0.25} l_p} \right)^{\frac{1}{0.75}} \times \frac{1}{eU} \quad (1)$$

where, n_i is the ion density, I is the current, ε_0 is the permittivity of free space, μ_i is the ion mobility, V_b is the probe bias, r_p is the probe radius, l_p is the probe length, e is the elementary charge, and U is the flow velocity.

3. Chemi-ionization reaction mechanism development

The reaction mechanism for the combustion of ethanol-air flame involving neutral species is used as the base mechanism, and it is improved to predict the ions and electrons distributions. In this work, the detailed mechanism presented by Marinov [18] for high temperature ethanol combustion, which contains 57 neutral species including nitrogen and 383 reactions, is used to describe the chemistry of neutral species. This mechanism is then combined with a set of ionic reactions to account for the charged species chemistry. It is assumed that the concentration of any neutral species present in the mechanism is much larger than the concentrations of charged species [25]. It means that the production and consumption of charged species may have little impact on the neutral species distributions.

For the kinetics of charged species, a mechanism involving 40 ionic reversible reactions and 6 charged species (HCO^+, H_3O^+, e^-, O_2^-, O^- and OH^-) [25] was adopted in the present model. Due to the lack of specific data for the ion chemistry in ethanol flame, the reaction of charged species from the methane flame was used as a reference. The reaction mechanisms of charged species developed in hydrocarbon flame were proposed in the works [12,24,32,33]. These works provided the important databases on the chemical processes of ions in the flame. The reaction mechanism of charged species considered in the present model is shown in Table 1. An improved reaction mechanism for predicting the charged species in the ethanol-air flame is obtained. The present model consists of 64 species and 423 reactions, and nitrogen is included in these species.

The chemistry solver Chemkin Pro is used for testing predictions of the present model and also conducting the reaction pathway analysis and sensitivity analysis to validate and analysis the ethanol combustion mechanism involving charged species. The National Aeronautics and Space Administration (NASA) database [34] and Burcat's database [35] are used to calculate the thermodynamic data for the species inside the ethanol-air flame. The transport coefficient is obtained and calculated from the mechanism of Marinov [18]. The Diffusion Opposed-flow Flame (OPPDIF code) is examined in this study. The initial temperatures of fuel and air are given as 350 K and 300 K, respectively. The pressure is given as 1 atm. For comparison analysis, temperature and pressure settings in the present model are consistent with the experimental condition [19], where the diffusion flames in a counterflow geometry was investigated. The Cylindrical coordinates is used. The total axial position is 12 mm, and the number of uniform grid points is 10.

4. Results and discussion

4.1. Temperature and neutral species profiles

The temperature predicted by the present model is compared to the experimental and numerical data of Saxena et al. [19] and the prediction of Marinov's mechanism [18] and it is shown in Fig. 2. The distance indicates the axial distance from the fuel side outlet to the air side. The maximum relative error of temperature between the present model and experiment is 4.4% and the maximum relative error of temperature between the present model and Marinov's model is 0.07%. The maximum temperature predicted by the present model is the same as the numerical data of Saxena, except the locations of the maximums