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The effect of hydrogen addition on premixed laminar acetylene–hydrogen–air and ethanol–hydrogen–air flames

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ARTICLE INFO

ABSTRACT

In the present work, the laminar premixed acetylene–hydrogen–air and ethanol–hydrogen–air flames were investigated numerically. Laminar flame speeds, the adiabatic flame temperatures were obtained utilizing CHEMKIN PREMIX and EQUI codes, respectively. Sensitivity analysis was performed and flame structure was analyzed. The results show that for acetylene–hydrogen–air flames, combustion is promoted by H and O radicals. The highest flame speed (247 cm/s) was obtained in mixture with 95% H_2–5% C_2H_2 at $\lambda = 1.0$. The region between $0.95 < X_{H2} < 1.0$ was referred to as the acetylene-accelerating hydrogen combustion since the flame speed increases with increase the acetylene fraction in the mixture. Further increase in the acetylene fraction decreases the H radicals in the flame front. In ethanol–hydrogen–air mixtures, the mixture reactivity is determined by H, OH and O radicals. For $X_{H2} < 0.6$, the flame speed in this regime increases linearly with increasing the hydrogen fraction. For $X_{H2} > 0.8$, the hydrogen chemistry control the combustion and ethanol addition inhibits the reactivity and reduces linearly the laminar flame speed. For $0.6 < X_{H2} < 0.8$, the laminar flame speed increases exponentially with the increase of hydrogen fraction.

1. Introduction

Several studies had been performed to study the flame characteristics of different fuels and combustible mixtures in order to find methods to reduce pollutant emission, improve the efficiency of combustion equipment and to utilize renewable energy sources such as biogas and hydrogen, as alternative fuels. These studies focus mainly on experimental and/or numerical work for measuring and predicting the flame structure, laminar flame speed, the adiabatic flame temperature, ignition delay and evaluating flame emissions

(CO, CO_2, unburned hydrocarbon, soot and NO) under different operating conditions and for distinct fuel mixtures.

Hydrogen–hydrocarbon blends are receiving attention as alternative fuels in power generation and stationary systems as well as automotive industries. This is because hydrogen is environmental friendly gas which produces only water when it is burnt. It has a very high combustibility, high flame speed with wide flammability limits [1–4] (LFL = 4.0% by volume, UFL = 76.5% by volume [5]) and thus has a great opportunity to improve performance, extend operability ranges and reduce pollutant emissions of lean combustion in both stationary

[6–12] and mobile [13–17] systems when it is added to hydrocarbon fuel (such as methane diesel and gasoline). Such partially replacement of hydrocarbon fuel with hydrogen could be a first step toward the large-scale economical introduction of hydrogen into the energy infrastructure for stationary and for transport systems [18–21].

However, since the combustion properties of hydrogen differ in many aspects from those of hydrocarbon fuels gas, the allowable fraction of hydrogen in gas mixtures may be limited by the deteriorating performance of gas combustion equipment such as spark-ignited engines, burners and turbines to hydrogen-enriched fuel.

Laminar flame speed is one of the most important physiochemical properties that characterize the combustion of a fuel. It embodies the fundamental information on diffusivity, reactivity, and it directly determines the rate of energy released during the combustion of a given combustible mixture. According to Tanford [22], who put forward a theory of burning velocity, the flame speed or the rate of flame propagation is controlled by the diffusion of atoms and radicals from the burned gas, and the rate at which these active species react with the unburned fuel.

Simulations of the premixed hybrid flames have been performed extensively [16,23–31]. Most of these computations were carried out with laminar premixed flame codes (CHEMKIN [32] or COSILAB [33]) utilizing detailed kinetic schemes [34,35]. In Law and Kwon [16], investigations were perform to measure and predict the laminar burning velocities of hydrocarbon–hydrogen–air flames in order to quantify the extent of burning rate reduction due to hydrocarbon addition to study the potential of improving hydrogen safety and engine performance by adding hydrocarbons to hydrogen–air mixtures. Sarli and Benedetto [36] used the CHEMKIN PREMIX code with the GRI kinetic mechanism to calculate the laminar burning velocities of hydrogen–methane/air mixtures at NTP conditions. The air ratio and the fuel composition were varied from lean to rich and from pure methane to pure hydrogen, respectively. The effects of radicals interactions were investigated and a correlation for the laminar burning velocity at different values of equivalence ratio and hydrogen content in the fuel were obtained. The results showed that the hydrogen addition enhances the methane slightly reactivity in lean mixtures, while at rich conditions a strong inhibiting effect of the hydrogen substitution by methane was observed.

In Huang et al. [37] laminar flame speeds simulations of neat primary reference fuels (PRFs), n-heptane and isooctane, PRF blends, reformer gas, and reformer gas/isooctane/air mixtures were performed using the Sandia PREMIX code in conjunction with CHEMKIN [32] and TRANSPORT [38] packages. The computations use windward differencing on the convective term, and include the thermal diffusion of H and H_2. Results demonstrate that the flame speeds of hydrocarbon/air mixtures increase with addition of a small amount of reformer gas, and the flame speeds of reformer gas/air mixtures are dramatically reduced with addition of a small amount of hydrocarbon fuel. Yufei et al. [39] performed measurement for laminar flame speeds, of CH_4 and C_2H_6 with H_2, O_2, N_2 and He, through digital particle image velocimetry. Additionally, in their work the PREMIX code was used for calculating the laminar flame speeds. In Law and Egolfopoulos

[40], thermal radiation from CH_4, CO, CO_2, and H_2O was considered for kinetic analysis with GRI-Mech 3.0 [34].

Erjiang Hu et al. [41,42], studied the laminar burning velocity and the characteristics of premixed methane–hydrogen–air flames. In their work, sensitivity analysis and flame structure were performed. It was found that the laminar burning velocity increases with the hydrogen fraction and the peak value of the laminar burning velocity shift to the rich mixture side.

Additionally, the laminar burning velocity of hydrogen–methane/air premixed flames has been experimentally measured at different values of equivalence ratio and fuel composition [43–48]. The reported results lead to a clear conclusion that the laminar burning velocity of hydrogen–methane flames increases with increasing hydrogen fraction in the mixture [2,36,49].

Haiyan et al. [5], studied the flammability limits of hydrogen-enriched natural in a constant volume combustion chamber supported with a high-speed schlieren photographic system. Correlations for both the lower and upper flammability limits of methane–hydrogen mixtures were reported. Moreover, in automotive industries, several research have been conducted to study the influence of using hydrogen in spark ignition engines [50–54].

Ethanol (CH_3CH_2OH) is a very important energy carrier that can be produced from renewable energy sources. It is becoming widely used directly in stationary and automobile systems [55,56]. However, it has a high latent heat of vaporization, low diffusivity and shows ignition difficulty at low temperature [54,57]. These disadvantages result in incomplete combustion.

On the other hand, acetylene is receiving a considerable growing interest in applications where high temperature flames are required. This is because acetylene, in comparison with other hydrocarbon fuels, has higher adiabatic flame temperature, high burning speed and small quenching distance (0.76 mm at atmospheric conditions [58]). Moreover and due to its high specific energy values it can be used in combustion-based power generation system for replacing electrochemical batteries and in combustion-based micro-sized power supply [58,59].

Due to the high autoignition temperature of hydrogen (approximately 858 K [60]), it has been widely recommended and proved to be an alternative fuel that can be applied on vehicles [61,62]. It has been proved to extend the lean limit of the fuel and shorten the periods during cold start and warm-up, and hence problems of cold fuel evaporation can be avoided/solved and thus the specific fuel consumption of in engines can be reduced [63].

Additionally, it has been proved that the addition of hydrogen to hydrocarbon fuels, reduces NO_x emissions [12,41,42,64], due to the decrease of the maximum combustion temperature via lean burning [63–68], and CO emissions due to the high reactivity of H_2 due to the higher concentration of OH radicals produced in the flame zone as a result of hydrogen addition [69].

In the present study, the adiabatic flame temperature and the laminar flame speed of H_2–air and H_2–C_2H_2, H_2–CH_4 and H_2–CH_3CH_2OH mixtures is calculated using PREMIX of CHEMKIN tools. For the case of hydrogen–hydrocarbon mixtures, the mole fraction of H_2 is varied from 0.0% to 100% and at an air ratio ($\lambda = 1$).

The well-known kinetic scheme GRI-Mech 3.0 mechanism of Ref. [34] is used in the calculation of the H_2, H_2–CH_4 and