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Numerical study of the physical and chemical effects of hydrogen addition on laminar premixed combustion characteristics of methane and ethane

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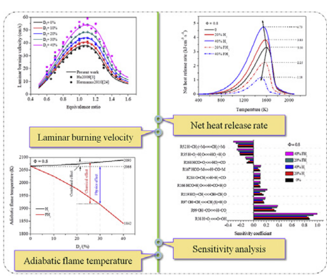
GRAPHICAL ABSTRACT



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ABSTRACT

Methane and ethane are taken as the research objects. Using H_2 as diluent, based on Chemkin II/Premix Code and modified detailed chemical reaction mechanism: GRI 3.0*-Mech (introducing three hypothetical substances of FH_2, FO_2 and FN_2), the physical and chemical effects of hydrogen on laminar burning velocities (LBVs), adiabatic flame temperatures (AFTs), net heat release rates (NHRRs) and elementary reactions responsible for temperature changes of two alkanes under different equivalence ratios were analyzed and determined. Results showed that the chemical effect of H_2 promotes the LBVs and ATFs of methane and ethane, while the physical effect decreases the two parameters. In addition, the physical effects of H_2 inhibit the chemical reactions of methane and ethane, resulting in the decrease of NHRRs. The chemical effect of H_2 accelerates the process of chemical reaction and obviously increases the NHRRs. The two most vital elementary reactions that promote the temperature rise of methane and ethane are $H + O_2 \Leftarrow\Rightarrow OH + O$ and $CO + OH$

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$<=>$ H + CO_2. The important reactions responsible for inhibiting the temperature rise are H + CH_3(+M) $<=>$ CH_4(+M) and H + O_2 + H_2O $<=>$ HO_2 + H_2O.

Introduction

Fuel combustion is the main way of energy acquisition. Policy and social pressures have led to a shift in energy structure towards cleaner and lower carbon. However, the main energy sources for decades to come still have to rely on biomass energy and traditional fossil energy, which mainly composed of hydrocarbon fuels. At present, natural gas (NG) is seen as the most potential clean alternative energy source among conventional energy sources and renewable energy such as coal, oil, natural gas and ethanol [1–5]. Main component of natural gas is methane (CH_4) and ethane (C_2H_6), and because natural gas is produced in different places, natural gas varies in composition ratio [6–8], for example, the proportion of methane in natural gas produced in Liaohe, China is 97.05%, while the natural gas in Abu Dhabi is mainly composed of 82% methane and nearly 16% ethane, and natural gas produced in the USA consists mainly of 85% methane and 14% ethane. In fact, the combustion of natural gas in air still produces atmospheric pollutants, such as soot and NOx [9,10]. Hydrogen Enriched Compressed Natural Gas (HCNG), also known as Hythane, is a feasible way to transfer to hydrogen energy. The mixture of natural gas and hydrogen can complement each other as engine fuel. Hydrogen addition improves the combustion performance of natural gas, reduces carbon emissions and broadens its ignition limit. The existence of natural gas makes up for the problems of fast combustion rate of hydrogen, low ignition energy and prone to premature ignition, deflagration and tempering.

Laminar combustion theory is the basis of studying turbulent combustion, and the combustion characteristics of laminar premixed combustion can directly reflect the essential characteristics of target fuel. For example, Laminar burning velocity (LBV) is the inherent characteristic of hydrocarbon fuel and an important parameter for laminar flame propagation and stability. Some researches [6,10] show that ethane blending into methane fuel can effectively enhance its laminar premixed combustion characteristics, such as laminar combustion speed, which may be one of the main reasons why laminar combustion speed of natural gas is faster than methane. There are two major reasons account for adding ethane can enhance LBV of methane. The first factor that the LBV of ethane is faster than LBV of methane [11,12]. With the increase of ethane doping ratio, the main fuel is changed from methane to ethane. Therefore, the laminar burning speed of the mixed fuel is increased. The other mainly point is that ethane will be cleaved into two methyl groups [13], which will greatly increase the concentration of important intermediate radicals and increase the reaction rate of HO_2+CH_3 $<=>$ OH + CH_3O and OH + CH_3 $<=>$ CH_2(S)+H_2O. These two reactions can promote the oxidation of methane, thereby improving the laminar burning velocity of methane. In recent years, many scholars have researched on the laminar combustion characteristics of methane and ethane.

Drrenberger et al. [6] utilized heat flux method (HFM) to measure the adiabatic LBVs of natural gas and C_1-C_4 alkanes flat flames under hydrogen doping ratio (0–40%), and summarized the correlations applied to LBV predictions of methane/ethane, methane-ethane mixtures and natural gas surrogate mixtures.

By HFM, Nilsson et al. [14] studied the LBVs of CH_4 mixed with C_2H_6, C_3H_8 respectively, and the LBVs of their binary/ternary mixtures mixed with hydrogen were also measured. It was found that the LBVs of CH_4 mixed with C_2H_6/C_3H_8 and their binary and ternary mixtures is higher than that of pure CH_4. Konnov's research group measured the non-stretching adiabatic LBVs of CH_4/N_2/O_2 [15], CH_4/O_2/CO_2 [16], C_2H_6/N_2/O_2 and C_2H_6/Ar/O_2 [17] in laminar premixed flames at different oxygen concentrations by HFM. The LBVs of stable flat flame of CH_4/O_2/CO_2 [18], C_2H_6/CO_2 /O_2 [19] and CH_4 (C_2H_6/C_3H_8)/CO_2 /O_2 [20] at a given oxygen concentration ranges (31.55–35%). Coppens et al. [21] experimentally and numerically analyzed the LBV and NO formation of methane doped with hydrogen in laminar premixed flame. In addition, Konnov et al. measured the adiabatic LBV of (CH_4+H_2)/N_2/O_2 at low pressure [22], and summarized and analyzed the influence of initial temperature on the LBVs of CH_4/N_2/O_2 and H_2/N_2/O_2 [23]. Hermanns et al. [24] and Coppens et al. [25] experimentally studied the effects of temperature and mixture composition on LBV and NO formation of (CH_4+H_2)/N_2/O_2. Goswami et al. also measured the LBVs of CH_4 at different pressures (1–5 atm) [26]. Then the LBVs of C_2H_6 and C_3H_8 at 1–4 bar were measured and compared [27]. Based on the accurate experimental results, the correlations between LBV and pressure were deduced. Hu et al. [3,28,29] and Wang et al. [4,30], based on spherical propagation flame (SPF), a systematical and numerical study had carried out the laminar premixed flame combustion characteristics of CH_4 under the condition of hydrogen addition. It was indicated that with the hydrogen doping ratios increasing, the non-stretching LBV and flame temperature increased, and the equivalence ratio of the maximum LBV also increased with the increasing of hydrogen content. The relationships between critical equivalence ratio for peak pressure rise rate and the ratio of H_2 in syngas (CO + H_2) and explosion characteristics of H_2 ratio in CH_4/H_2/Air has been experimentally studied by Sun [31,32]. Ren et al. [33–35] conducted numerical analysis on the effects of different hydrogen doping ratios on the laminar premixed combustion characteristics of natural gas and the effects of CO_2 and H_2O on the formation of intermediate H_2 in methane/air flame and effect of different N_2/CO_2/H_2O doping ratio in CH_4/air laminar combustion flame. Based on the experimental results, the dependence of the LBV of methane on the equivalence ratio was also emphasized by Ren et al. [33-35]. Zahedi et al. [36] analyzed the effects of N_2, CO_2 and H_2 on LBV and NO formation of CH_4 premixed flames by HFM and numerical simulation. Xiang et al. [37] performed a numerical analysis on the effect of CO_2 on intermediate important free radicals in methane laminar premixed flames. Bougrine et al. [38] used an detailed chemical reaction mechanism to predict the (CH_4+H_2)/air laminar combustion characteristics under high temperature and pressure condition. The numerical results showed that H plays an indispensable role in leading the main chemical reaction, what's more, adding hydrogen can promote the formation of the important intermediate radical H. Lafay et al. [39] carried out an experimental and numerical investigation on the laminar flame thickness of methane-air mixture with adding hydrogen. It was concluded that the thickness of the laminar flame is reduced by hydrogen addition. Li et al. [40] numerically studied the reaction kinetic mechanism and thermodynamic characteristics of laminar premixed flames of hydrogen-doped methane mixtures. The results reported that hydrogen addition promotes the heat release in the early stage of methane laminar flames and the reaction that hydrogen has the greatest impact on $OH + H_2 <=> H + H_2O$, which is the most important reaction for heat release. Ying and Liu [41] reported the dilution characteristics of the substance FH_2 which has hydrogen thermal and transport characteristics and it isn't involved into the chemical reaction by numerical simulation. The effects of 0–40% hydrogen doping on the specific chemical effects of premixed flame temperature, free radical concentration and NO emission of methane laminar flames were discussed. Li et al. [42] investigated the effects of hydrogen addition on the LBVs of CH_4, C_2H_6 and C_3H_8 based on the opposed-flow diffusion flame and numerical simulation. They discussed in detail the influence of adding hydrogen existence on the important reactions of LBVs of three fuels and the changes in the molar concentration of major free radicals. Halter et al. applied the classical shadowing method to study the LBV of methane/air at elevated pressure and hydrogen doping in a spherical flame [43]. The laminar and turbulent premixed flame of methane with hydrogen addition were studied by using SPF and pilot flame at high pressure, respectively [44]. In addition, Halter et al. [45] introduced FCO_2 and compared the effects of N_2 and CO_2 on LBVs of methane and iso-octane. Park et al. [46] used an detailed chemical reaction mechanism to study the methane/air counter-flow diffusion flame diluted by hydrogen and water vapor. It was found that the addition of a small amount of water vapor increased the maximum temperature of the flame, inhibited the formation of H and O free radicals, promoted the rise of OH free radical concentration and depressed the formation of NO. Recently, Amar et al. [47] carried out numerical studies on the counter-flow diffusion flame of BG75 (75%CH_4 and 25%CO_2)/H_2 mixture. Han et al. [48] conducted an experimental investigation on the LBVs of CH_4 and C_2H_6 at different temperatures by using HFM. The exponential coefficient correlation of the temperature dependence of LBV was deduced through the analysis of total activation energy. Besides, Liu et al. [49] numerically studied the exergy losses in CH_4/H_2 laminar combustion flame, the results showed that minimum exergy loss occurred at the equivalence ratio of 0.9 for different blends. Zhang et al. [50] studied the exergy losses in H_2 premixed flames with Ar/N_2/CO_2 as diluents, and numerical simulation results showed the thermal effects of diluents are the primary factor influencing the exergy loss.

Hu et al. [51] explored the effects of initial pressure on methane/air ignition delay and LBV were investigated using constant volume incendiary bombs, USC mech [52] and the Aramco mech [53], and summarized up the relationship between ignition delay time and laminar burning velocity. Cai et al. [54] experimentally and numerically investigated the effects of initial pressure on laminar burning velocity and Markstein lengths by using the spherical flame method and the Aramco mechanism [53]. Apart from that, Chen et al. [55] numerically studied the laminar burning velocity and flame structure of methane/ethylene/air mixtures, the results showed that the addition of ethylene increases the concentration of intermediate important free radicals O, OH, H.

From the above research review, it can be found that there are many studies on pure methane, hydrogen-doped methane and pure ethane, which are the most abundant in natural gas. However, the study of hydrogen doping in ethane combustion is rare, and especially, the effect of H_2 dilution on the physical and chemical characteristics of laminar premixed combustion of methane and ethane is still lacking. This work presents the results of the physical and chemical effects of hydrogen on LBVs, AFTs, NHRRs and elementary reactions responsible for temperature changes of methane and ethane under different equivalence ratios.

Numerical calculation and mechanism validation

In this article, the effects of different hydrogen doping ratios on the laminar premixed flames of methane and ethane were calculated by using the premixed free-propagating flame model based on Chemkin II [56]/Premix Code [57]. In the calculation process, the mixed gas flow rate is regarded as the eigenvalue of the solution of the premixed free-propagating flame, besides, its initial value is kept at 0.04 g/(cm^2·s). The multicomponent transport model is used in all operating conditions, and the Soret effect is taken into account. Using adaptive mesh (50 meshes), the maximum number of meshes is set to 500. Gradient GRAD = 0.04, curvature GURV = 0.04. Relative and absolute errors are set at 10^{-4} and 10^{-9} respectively in the iteration process. In order to achieve zero gradients for all variables, the one-dimensional computational domain boundary was set from -0.2 cm to 6 or 10 cm to achieve zero gradients for all variables, so that it can satisfy the requirements of simulation.

The formula for calculating the amount of hydrogen mixing is as follows.

$$D_1 = \frac{V_{diluents}}{V_{diluents} + V_{fuels}} \tag{1}$$

Where $V_{diluent}$ and V_{fuels} are volume fractions of hydrogen and fuel, respectively. D_1 represents the proportion of diluent in the fuel/diluent mixture and is generally used to study the effects of different fuel mixtures [40,47,48]. It can also be used to investigate the influence of impurity gases, such as CO_2 and N_2 in fuels (such as biogas) [31,42,58].

In order to select a precise and reasonable combustion mechanism, based on previous research results and previous work, two widely recognized kinetic mechanisms: GRI-Mech 3.0 [58] (containing 325 elementary oxidation and decomposition reactions and 53 species) and San Diego-Mech [59] of the latest revision (containing 268 elementary reactions and 57 species) that can be applied to oxidation combustion of methane and ethane were selected to analyze the laminar premixed combustion characteristics of the hydrogen addition of methane and ethane.

Moreover, to determine the physical and chemical effects of H_2, three hypothetical substances, FH_2, FO_2 and FN_2, were added to the GRI 3.0 and San Diego models. FO_2 and FN_2 are defined to eliminate the effects of H_2 on combustion chemical reactions of corresponding oxidant components [41]. Correspondingly, the three hypothetical substances have the same thermodynamic and transport properties of H_2, O_2 and N_2 respectively, and they are not involved into any chemical reaction and do not play any role in cracking molecules, but only affect the combustion chemical reaction process through dilution effect, specific heat release and three-body collision, just like inert gases. Therefore, the number of elementary reactions in the two mechanisms cannot increase, nor does it affect the calculation results. The modified models of GRI 3.0 mech and San Diego are defined as GRI 3.0* and San Diego*, as shown in Table 1.

To verify the rationality and accuracy of the mechanism selected in this paper, Fig. 1 compares the simulation results of LBVs of methane and ethane at 298 K and 1 atm with other scholars experimental results in relevant literature [3,6,14,15,17,21,25,28,42,44,48,60–72].

From Fig. 1 (a), it can be seen that the LBVs of CH_4 calculated by GRI 3.0* mechanism agrees well with the experimental values at different equivalence ratios. The results from San Diego* mechanism prediction agree with the experimental values at lean conditions, but are much smaller than the experimental values at stoichiometric and rich conditions. Fig. 1 (b) shows that the general trend of C_2H_6 results simulated by GRI 3.0* and San Diego* mechanism is consistent with the experimental values, but the prediction of San Diego* mechanism is slightly larger than the experimental values at lean combustion and less than the experimental values at rich condition. Thus, compared with the experimental results, the CH_4 and C_2H_6 laminar premixed flames under the condition of different hydrogen doping ratios should be calculated by GRI 3.0* mechanism.

Results and discussion

LBV and AFT at various initial temperatures and pressures

Generally, in industry, before the fuel enters the combustion chamber for combustion, the waste heat generated in the industrial system will be used to preheat the fuel and oxidant in order to save energy and improve the thermal efficiency in fuel combustion. In addition, combustion in internal combustion engine is carried out under high temperature and pressure. Studying laminar premixed combustion of methane and ethane under different initial pressures is helpful to understand the influence of initial parameters on laminar premixed combustion and provide data reference and experimental guidance for combustion in engine cylinder. Fig. 2 gives the LBVs and AFTs of methane and ethane vary with the equivalence ratios at different initial pressures with the initial temperatures 298 K and 473 K, respectively.

Table 1 – Comparison of GRI 3.0 and San Diego mechanism before and after modification.

Mechanism	Species	Elemental reactions
GRI 3.0	53	325
GRI 3.0*	**56**	**325**
San Diego	57	268
San Diego*	**60**	**268**

The experimental values [26,69] of LBVs of methane and ethane at 298 K, 1, 2 and 5 atm are given in Fig. 2 (a1) and (a2). From Fig. 2 (a1), it is seen that the calculated values of CH_4 at 298 K at different initial pressures agree well with the experimental values measured by HFM [26]. The calculated LBVs of C_2H_6 in Fig. 2 (a2) at room temperature and pressure is in good accordance with the experimental data measured via the counter-flow flame method [71]. When the initial pressure is 2 and 5 atm, the calculated value is slightly overpredicted. Besides, in Fig. 2 (a1) and (a2), it can be found that the LBVs of methane and ethane increase with the increasing of initial temperature, and firstly increase and then decrease with the increase of equivalence ratios. The equivalence ratio of the

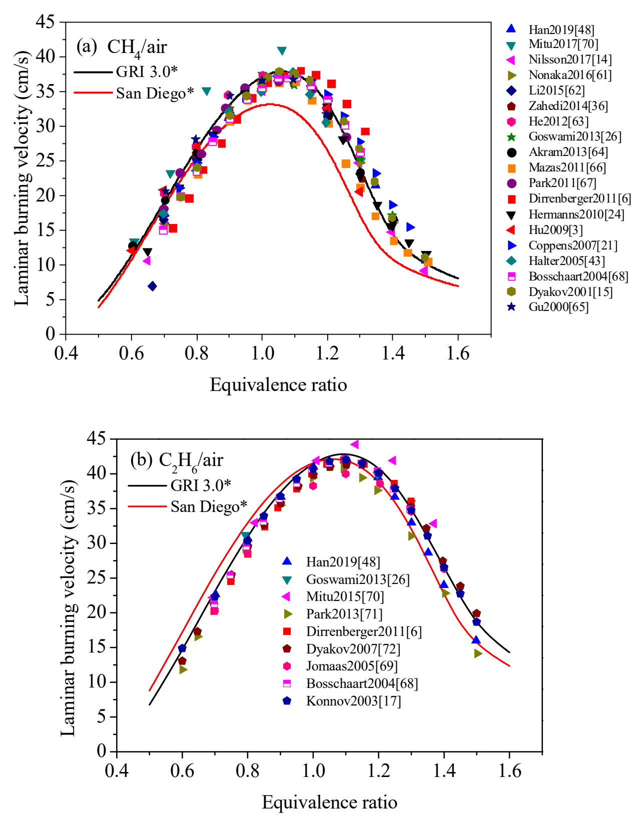

Fig. 1 – Experimental and simulated LBVs at 298 K and 1 atm. (a) CH_4/air; (b) C_2H_6/air. (Symbols: experimental data; lines: simulated data).

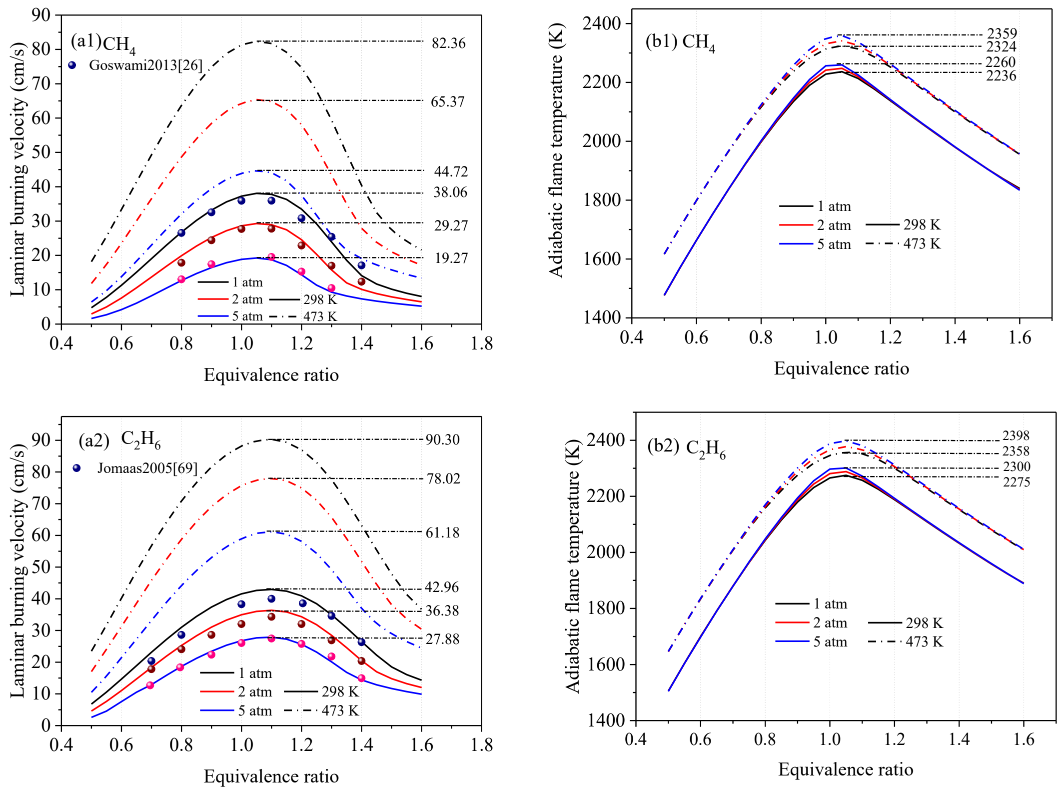

Fig. 2 – Simulated LBVs and AFTs with various initial temperature and pressures.

maximum LBV of CH_4 at different initial temperatures is 1.05, while that of C_2H_6 is 1.10. Moreover, the LBV of C_2H_6 is larger than that of CH_4. With the initial temperature changed from 298 K to 473 K, the LBV of methane and ethane increases by approximately two time.

Fig. 2 (b1) and (b2) show that the AFTs of methane and ethane vary with the equivalence ratio and initial temperature, and the variation trend is consistent with the LBV, but the difference is that the equivalence ratio corresponding to the maximum AFT of two alkanes is 1.05, reflecting the equivalence ratio of the maximum AFT and LBV of C_2H_6 is different. The AFT of C_2H_6 is higher than that of CH_4. When the initial temperature rises from 298 K to 473 K, the AFT of methane and ethane increases by 88 K and 86 K, respectively.

In addition, it can be concluded that from Fig. 2 (a1) and (a2), the LBVs of the two fuels decrease with the increase of pressures at the same temperature. The higher the initial temperature is, the more obvious the effect of pressure on the decrease of LBV is, and the decreasing LBV of CH_4 is the largest when the pressure increases. At the same temperature, the pressure increases from 1 to 5 atm, and the LBV of CH_4 decreases to one-half of the original, while C_2H_6 decreases to about three-fifths.

It can be concluded from Fig. 2 (b1) and (b2) that the increase of pressure promotes the increasing of AFTs of methane and ethane. For the ranges of equivalence ratios are from 0.8 to 1.2, the change of initial pressure has the significant effect on the AFTs. The higher the initial temperature is, the more obvious the pressure increases the AFT. This is because the increasing of pressure enhances the collision reaction of activating molecules, while the increasing temperature promotes the cracking of fuel and accelerates the combustion reaction rate, thus increasing the adiabatic flame temperature. It is noteworthy that the change of initial pressure does not affect the corresponding equivalence ratio of maximum LBV and AFT.

Effect of hydrogen addition on LBV

Comparison on the results of LBV of CH_4 with hydrogen addition

From the first section, we can see that in recent years, domestic and foreign scholars have done a lot of research on CH_4 combustion. Due to the application of natural gas in internal combustion engines, accurate measurement and calculation of LBV of CH_4-H_2 mixture has become a hot topic in recent years. Fig. 3 is a comparison of the calculated LBV of CH_4 with H_2 addition at room temperature and pressure with the experimental results of Hu et al. (0.1 MPa, 303 K) [3] and Hermanns et al. (1 atm, 298 K) [24]. It can be seen from Fig. 3 that the calculation results of LBVs of CH_4 doped with H_2 are in accord well with those measured by using HFM from Hermanns et al. [24]. Only when the hydrogen ratio is 40%, the calculated value is slightly smaller than that in the laboratory, and overpredicts slightly at rich conditions, but the overall trend is consistent. Due to the inconsistency between the calculation conditions and the results in Hu et al. [3] when measuring SPF with constant volume bomb, the calculated values conforms to the measurements without the hydrogen addition and with hydrogen doping ratio is 20%. When the hydrogen doping ratio is more than 20%, the experimental values are much larger than the calculated values. Compared with the experimental values of LBVs measured by two methods, it can be further proved that the calculated results in this paper can accurately predict the laminar combustion characteristics of methane and ethane. As shown in Fig. 3, the LBV increases with the increasing of hydrogen content in CH_4/H_2, and the larger the hydrogen doping ratio is, the greater the increase of LBV is. In addition, with the increase of hydrogen doping ratio, the equivalence ratio corresponding to the maximum LBV increases. When the hydrogen doping ratio is less than 20%, $\Phi = 1.05$, and when the D_1 is more than 20%, $\Phi = 1.10$, which is consistent with the results obtained in Ref. [3]. The influence of hydrogen existence on the LBV of CH_4 in the rich combustion zone is greater than that in the lean.

The laminar premixed combustion characteristics of fuels are usually affected by mixed combustion of diluents in three ways: (1) the dilution effect due to the decrease in the concentration of the fuel combustion reaction substance with the addition of the diluent; (2) the thermal effect due to the change in the flame temperature; and (3) the chemical effect due to the participation of the diluent in the relevant combustion chemical reaction. In the actual combustion process, these three effects occur simultaneously and are tightly coupled. In this paper, the combined effect of dilution effect and thermal effect on laminar premixed combustion characteristics is defined as "physical effect". Therefore, the role of the diluent in the combustion chemical reaction is mainly contributed by both physical and chemical effects. The chemical effect of H_2 on the LBV can be expressed as follows.

$$\Delta S_{L,Chem} = S_{L,FH_2} - S_{L,H_2} \tag{2}$$

Where S_{L,FH_2} and S_{L,H_2} are the LBV of mixed gas with FH_2 and H_2 addition, respectively. The difference $\Delta S_{L,Chem}$ between the two represents the effect of the chemical reactivity of H_2 on the LBV.

The physical effect of H_2 on LBV can be expressed by:

$$\Delta S_{L,Phys} = S_{L,0} - S_{L,FH_2} \tag{3}$$

Where $S_{L,0}$ is the LBV of the mixed gas without H_2 addition. The difference $\Delta S_{l,Phys}$ represents physical effect of H_2 on the LBV.

If $\Delta S_{L,Chem}$ and $\Delta S_{l,Phys}$ are positive, the chemical and physical effects of H_2 decrease the LBV. Conversely, the LBV is increased. The specific effect of methane and ethane blending H_2 on the LBV is represented by the following formula

$$\Delta S_L = \Delta S_{L,Chem} \Delta S_L, Phys = \Delta S_{L,0} - S_{L,H_2} \tag{4}$$

Where ΔS_L indicates the specific effect of blending H_2 on the LBV of the laminar flames of methane and ethane. If it was positive, hydrogen addition would reduce the LBV, and if it was negative, the LBV would be increased.

Figs. 4 and 5 illustrate the simulation results of LBVs of CH_4 and C_2H_6 with and without H_2 and FH_2 addition at 398 K and 1 atm (The calculations are based on this initial temperature and pressure unless otherwise specified) under lean ($\Phi = 0.8$), stoichiometric ($\Phi = 1.0$), rich ($\Phi = 1.2$) combustion conditions.

It can be observed from Fig. 4 (a) that the calculated values of CH_4 doped with hydrogen agree well with the experimental values [24] with the change of hydrogen doping ratio at $\Phi = 0.8$. The LBV of CH_4 is greatly increased by hydrogen addition, and enhanced by the chemical effect of H_2. The LBV decreases with the physical effect of H_2. The chemical effect of H_2 is twice that of physical effect, so the overall effect of hydrogen doping is to increase the LBV. As shown in Fig. 4 (a)–(c), the chemical effect of H_2 on LBV increase and the decrease on LBV for H_2 physical effect are enhanced with the increase of hydrogen doping ratios and equivalence ratios.

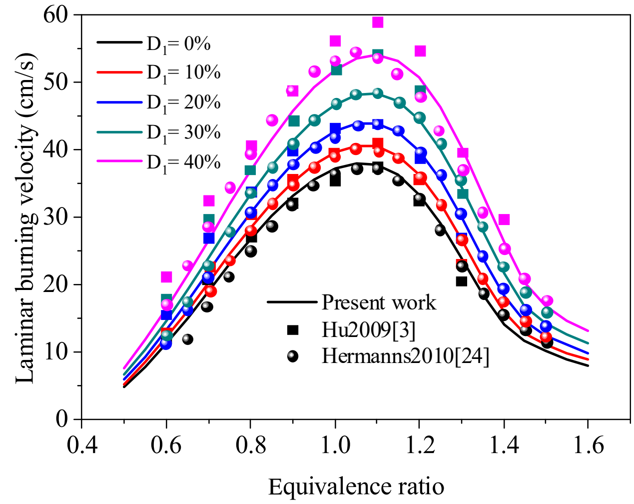

Fig. 3 – Comparison of simulation and experimental results of LBV of CH_4 with hydrogen addition.

From Fig. 5, it is found that the chemical and physical effects of H_2 addition on the LBV of C_2H_6 are consistent with those of CH_4. That is to say, the chemical effect of H_2 promotes the LBV of C_2H_6 to increase, while the physical effect reduces the LBV. The effect of H_2 decreases with the increase of carbon atom number of alkanes [59]. This is mainly due to the high molecular weight of alkanes with more carbon atoms. At the same hydrogen doping ratio, the proportion of H_2 in the mixture decreases, resulting in the decrease of the combustion chemical dynamic effect. According to literature [3], when the hydrogen doping ratio reaches more than 60%, the main fuel in CH_4-H_2 mixture will become H_2, meaning that the combustion characteristics of fuel will turn to H_2, and the participation of CH_4 will limit the rapid diffusion of H_2 combustion.

Effect of H_2 and FH_2 on AFT

The influence of physical and chemical effects of H_2 on the AFT and NHRR in the laminar premixed flame of methane and ethane can also be expressed by formulas (2) and (3). It is only necessary to change the laminar combustion parameters in the formulas into corresponding research parameters (such as AFT, NHRR, molar fraction of substance, etc.).

Figs. 6 and 7 show the effects of physical and chemical effects of H_2 on the AFTs of methane and ethane under lean, stoichiometric and rich conditions. As shown in Figs. 6 (a) and 7 (a), the physical and chemical effects of H_2 on the AFT are similar to that of LBV. The difference is that the addition of H_2 has little effect on the rise of AFT, and the physical and chemical effects have little difference. But the combined effect makes the final temperature rise slightly.

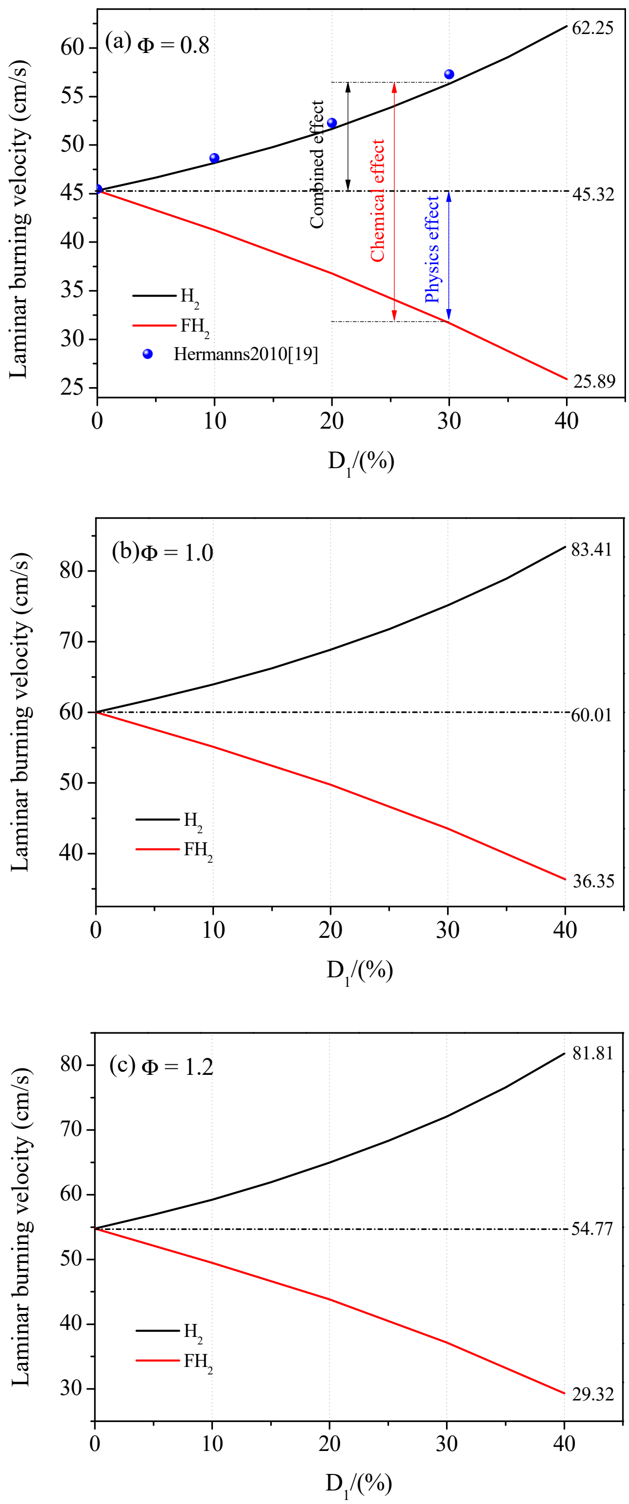

Fig. 4 – LBVs of CH_4 with H_2 and FH_2 addition at different equivalence ratios.

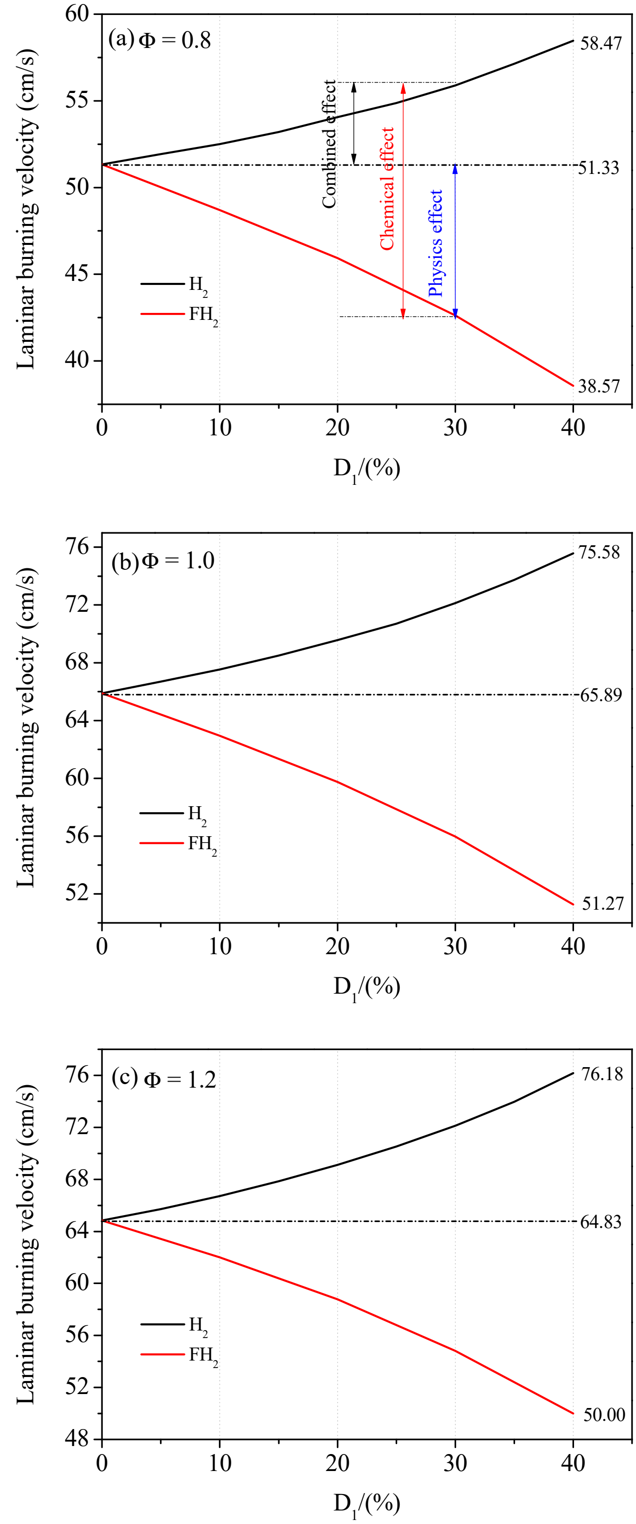

Fig. 5 – LBVs of C_2H_6 with H_2 and FH_2 addition at different equivalence ratios.

Compared with Figs. 6 and 7, it is found that the AFT of methane and ethane increases with the increasing of hydrogen doping ratio. Under the same equivalence ratio, the physical and chemical effects of H_2 on the AFT also decrease with the increase of the number of carbon atoms. The chemical effect of H_2 plays a pivotal role in the increase of AFT. The main reason is that H_2 participates in chemical reactions to increase the molar concentration of active free radical pools (O, H, OH, etc.) during combustion process, thus expanding the branched chain reaction in combustion and accelerating the combustion reaction rate [40,58]. In addition,

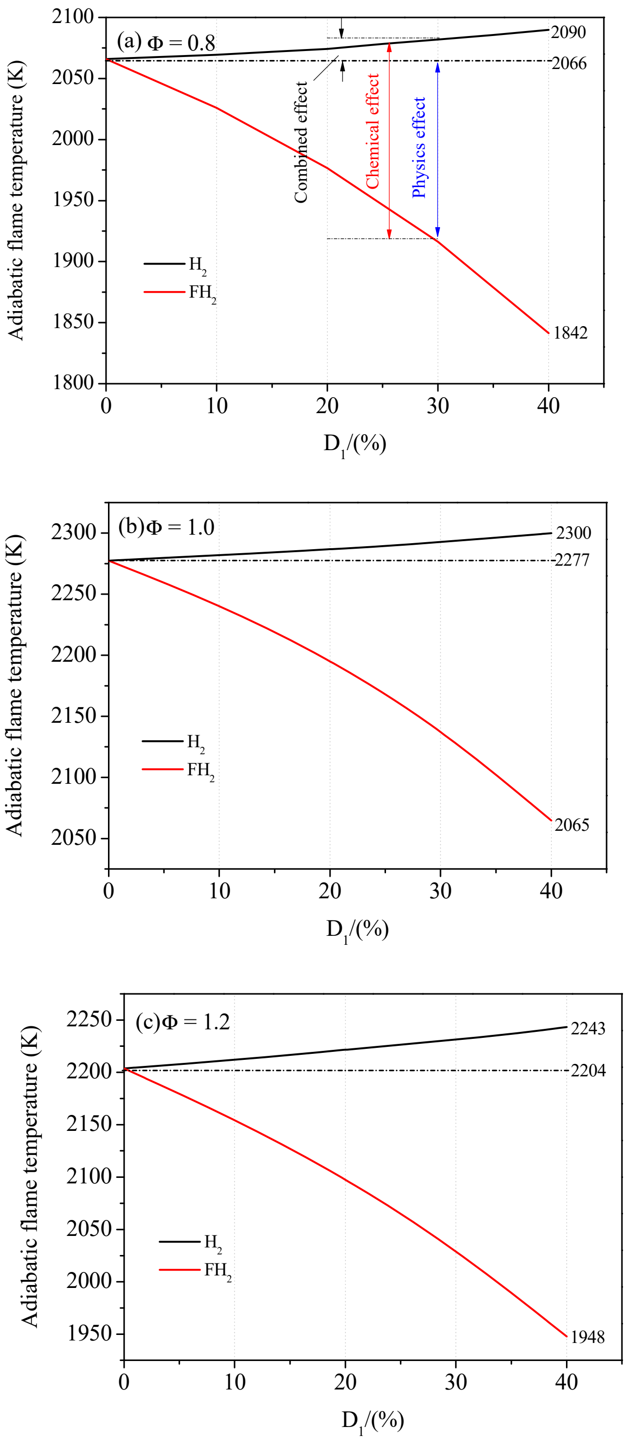

Fig. 6 – AFTs of CH_4 with H_2 and FH_2 addition at different equivalence ratios.

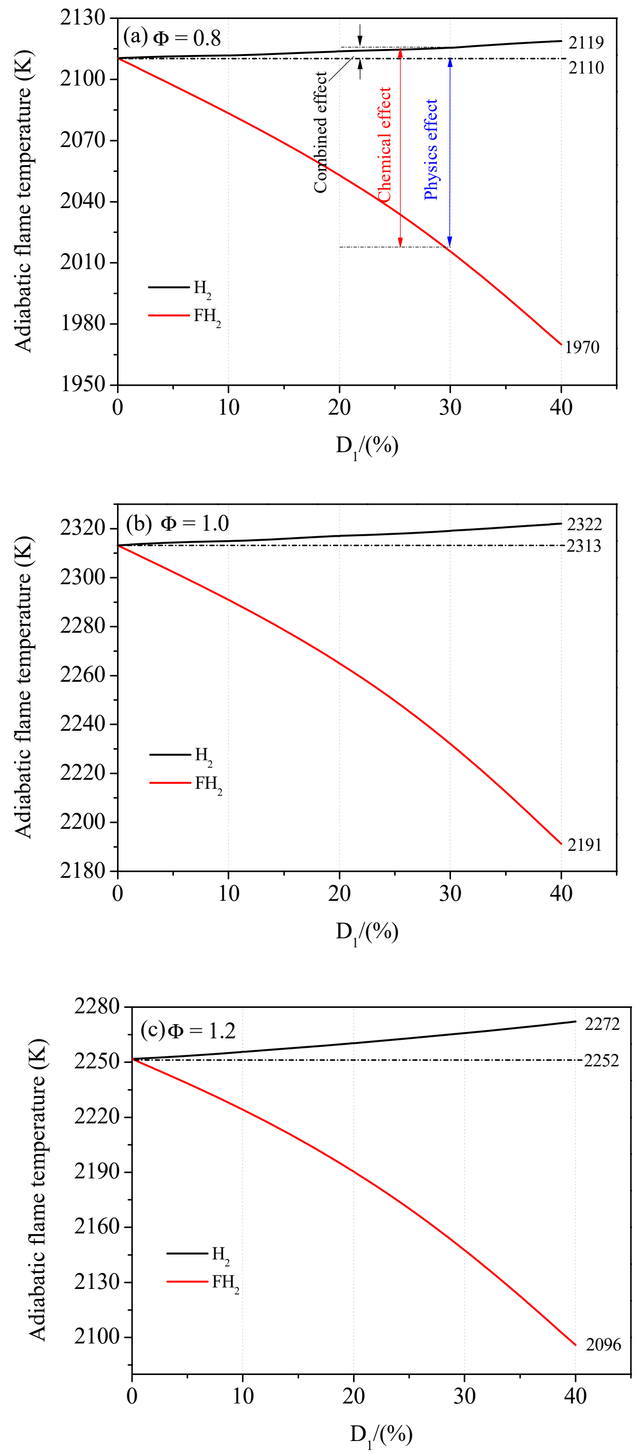

Fig. 7 – AFTs of C_2H_6 with H_2 and FH_2 addition at different equivalence ratios.

for the same fuel, the physical and chemical effects of H_2 have the greatest impact on LBV and AFT under the rich condition, and the least impact on the stoichiometry. In addition, the addition of H_2 increased the AFT of CH_4 most obviously, and the increase of temperature was several times of that of ethane at the same equivalence ratio.

Effect of H_2 and FH_2 on NHRR

As one of the important parameters of laminar combustion characteristic, researching on the heat release rate of fuel has many important implications. For instance, studying the NHRR of fuel has reference value for the later application in internal combustion engines. The NHRR affects the ignition delay time of the fuel and the design of the internal combustion engine. Besides, the NHRR reflects the amount of energy released by the combustibles in the fire, and the heat release rate of various combustibles is the basis for dividing the fire resistance rating of the building materials, and is an important prerequisite for fire protection design and fire risk assessment. Thus, NHRR comparison has great significance for the future application of fuel. The NHRR reflects the heat generation per unit time in the combustion process, that is, the speed or intensity of chemical reaction in the combustion process. The more intense of the chemical reaction is, the faster the chemical reaction rate is. And the higher the LBV and the AFT are, the higher the NHRR is.

Figs. 8 and 9 show the NHRR of methane and ethane varied with temperature at diverse equivalence ratios and hydrogen doping ratios of 0%, 20% and 40%. It can be found that NHRRs of methane and ethane enhances with the increasing of D_1. From Figs. 8 (a) and 9 (a), the flame temperature corresponding to the peak NHRRs decreases with the increase of hydrogen doping ratio when the equivalence ratio is 0.8. That is because with the D_1 increases, the flame combustion reaction begins at a position closer to the nozzle, and the combustion reaction takes place at a lower temperature, indicating that hydrogen doping accelerates the combustion reaction rate. As the hydrogen doping ratio increases, the physical effect of H_2 decreases. Obviously, as the NHRR decreases gradually, the flame temperature corresponding to the peak value decreases gradually. Combined with Effect of H_2 and FH_2 on AFT, the physical effect of H_2 on the temperature drop of AFT is discussed. The physical effect of H_2 inhibits the combustion chemical reaction resulting in the decrease of NHRR. The chemical effect of H_2 accelerates the process of chemical reaction and obviously increases the NHRR of laminar premixed combustion of methane and ethane. At the same equivalence ratio, hydrogen addition has the greatest influence on CH_4. Moreover, when methane and ethane are mixed with hydrogen, the increase of NHRR is more obvious in the case of rich combustion.

Effect of H_2 and FH_2 on sensitivity analysis

The most forceful and systematic method to quantitatively study the relationship between the model and its parameters is sensitivity analysis. For combustion problems, this method can greatly improve people's insight into the importance of various reaction pathways, so as to achieve the goal of combustion control. In present work, sensitivity analysis was applied to research on the effect of difference hydrogen doping ratio on the temperature of laminar premixed flames of methane and ethane. A more direct understanding of the effects of individual elementary reactions on combustion temperature is conducted. It is of great significance to understand heat release characteristics, to simplify reaction models and to determine control methods. The following formula is used for sensitivity analysis in this paper.

$$c_i(t, l + \Delta l) = c_i(t, l) + \sum_{i=1}^{56} \frac{\partial c_i}{\partial l_j} \Delta l_j + ... \quad (5)$$

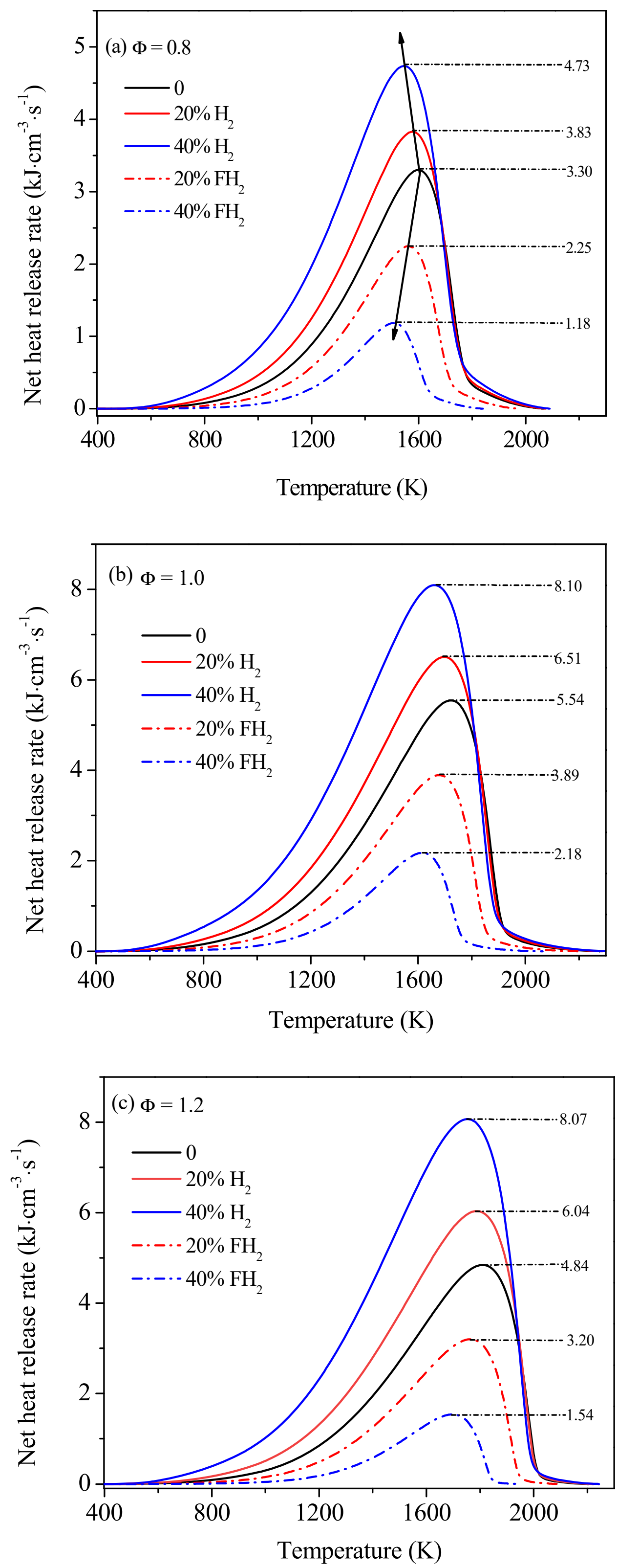

Fig. 8 – NHRRs of CH_4 with H_2 and FH_2 addition at different equivalence ratios.

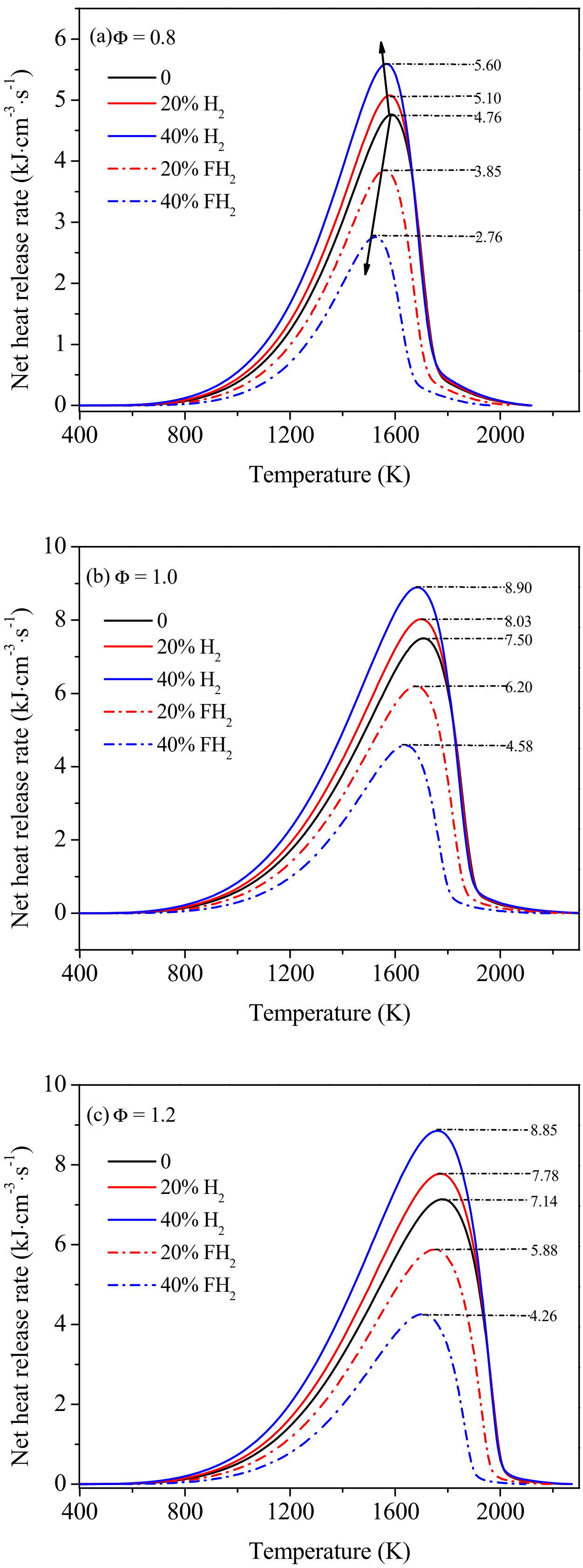

Fig. 9 – NHRRs of C_2H_6 with H_2 and FH_2 addition at different equivalence ratios.

Where i is the species i (56 species) and c is the concentration. l is the distance from the nozzle, $\partial c_i/\partial c_j$ is the first-order sensitivity coefficient. So as to study the laminar premixed combustion characteristics of methane and ethane, the first-order sensitivity coefficient of AFT was used to analyze the importance of elementary reactions to laminar premixed flame temperature.

Fig. 10 shows the sensitivity coefficients of CH_4 temperature with H_2 and FH_2 addition at different equivalence ratios. It can be found that in Fig. 10, the most important reaction that promotes the increasing of temperature at different equivalence ratios is R38 H + O_2 <=> O + OH. It is the most critical elementary reaction in laminar premixed combustion of CH_4 and the initial elementary reaction of branched chain reaction in combustion [39,40,58]. R38 continuously produces active free radicals during the combustion process and promotes the chain reaction, which largely determines the overall combustion reaction rate. With the increasing of D_1, the dominant effect of R38 on the temperature rise of CH_4 decreases. This is because H_2 participates in combustion chemical reaction and promotes the formation of active free radicals. By comparing with the sensitivity of FH_2 blending, it can be found that H_2 does not participate in chemical reactions, which greatly increases the dependence of temperature rise on R38. The primary reaction that plays a leading role in inhibiting temperature rise is R52 H + CH_3(+M) <=> CH_4(+M). The positive direction of R52 is a chain termination reaction, which hinders the development of chain reaction, reducing the combustion reaction rate and inhibiting the temperature rise. With the increasing of hydrogen doping ratio, the effect of R52 on inhibiting temperature rise is weakened, and the dominant effect of FH_2 is increased.

Compared with Fig. 10 (a)–(c), hydrogen addition can increase the inhibition of R35 H + O_2 + H_2O <=> HO_2 + H_2O on temperature rise at $\Phi = 1.0$ and enhance the promotion of R284 O + CH_3 <=> H + H_2+ CO on increasing temperature when the equivalence ratio is 1.2. In other cases, hydrogen doping decreases the sensitivity of important reactions to temperature changes in CH_4 laminar premixed combustion, while FH_2 addition gradually increases the dependence of temperature on the reactions.

The first three elementary reactions which promote and inhibit the rise of CH_4 laminar premixed combustion temperature are different under different equivalence ratios. When the equivalence ratio is 0.8, the first three elementary reactions in the promotion of temperature rise are R38 H + O_2 <=> O + OH, R99 OH + CO <=> H + CO_2 and R97 OH + CH_3 <=> CH_2(S) + H_2O, the first three elementary reactions in inhibition are in turn R52 H + CH_3(+M) <=> CH_4(+M), R35 H + O_2 + H_2O <=> HO_2 + H_2O and R168 HCO + O_2 <=> HO_2 + CO. At $\Phi = 1.0$, the first three elementary reactions in the promotion effect of temperature rise are the same as those in lean combustion, while one of the elementary reactions for inhibition change from R168 to R55 H + HCO <=> H_2 + CO. When the equivalence ratio is 1.2, the first three reactions in the promotion for temperature rise are R38 H + O_2 <=> O + OH, R119 HO_2 + CH_3 <=> OH + CH_3O and R166 HCO + H_2O <=> H + CO + H_2O, while the reactions for the inhibition are R52, R55 and R158 $2CH_3$(+M) <=> C_2H_6(+M). When combustion changes from lean to rich conditions, the content of oxygen decreases

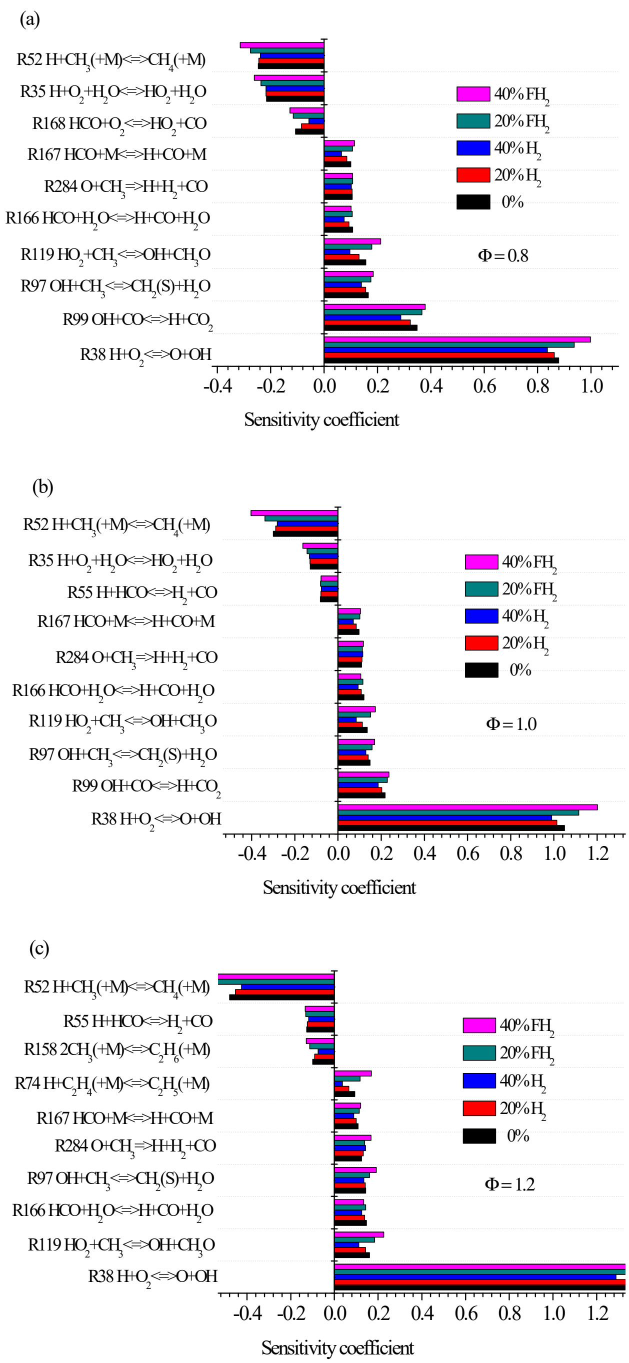

Fig. 10 – Sensitivity coefficients of CH_4 temperature with H_2 and FH_2 addition at different equivalence ratios.

relatively, and more CH_3 and H are produced by reaction cracking of CH_4 and H_2 in the combustion process, thus reacting with oxygen to produce important intermediate products HCO and CO in the oxidation combustion reaction of CH_4. Therefore, the elementary reactions with different equivalence ratios, which contribute significantly to the laminar premixed combustion temperature of CH_4, show the changes in Fig. 10.

When equivalence ratio≤1, with the increase of hydrogen ratio, the chemical effect of hydrogen on promoting effect of R38 and the inhibitory effect on R52 increase. This is because as the hydrogen doping ratio increases, the amount of methane decreases, and if hydrogen does not participate in the chemical reaction, methane has sufficient air for the oxidation reaction. The reaction rate of R38 is promoted and the faster decomposition rate of methane produces more H, which leads to the positive reaction rate of R52. However, physical effect always promotes the R38 and R52 reaction rate. When equivalence ratio>1, chemical and physical effects have little influence on the R38 reaction rate, which means with the increase of hydrogen doping ratio, chemical effect and physical effect have little influence on R38, while chemical effect gradually reduces the influence on R52, while physical effect no longer changes with the hydrogen doping ratio.

Fig. 11 gives the temperature sensitivity coefficients of C_2H_6 doped with hydrogen at different equivalence ratios. According to Fig. 11 (a)–(c), the most important reaction that promotes the temperature rise of C_2H_6 at different equivalence ratios is R38 H + O_2 <=> O + OH, the same as CH_4. The difference is that with the increase of D_1, at $\Phi = 0.8$, the effect of R38 on temperature rise first decreases and then increases. Under stoichiometric condition, hydrogen addition increases the promotion of R38, while at $\Phi = 1.2$, adding hydrogen decreases the promotion of R38. When the equivalence ratio<1, the influence of chemical effect and physical effect on R38 increases with the increase of hydrogen doping ratio. Because the adiabatic flame temperature increases with the increase of hydrogen, which increases the H generated by H_2 and ethane during the oxidation process, leading to the increase of hydrogen to promote the reaction rate of R38. When the equivalence ratio≥1, the chemical effect and the physical effect have little effect on R38 reaction rate. With the increase of hydrogen doping ratio, chemical effects on the inhibition of R52 and R159 reaction rate increase. On the contrary, the promoting effect of physical effect on R159 increases with the increase of hydrogen doping ratio.

In addition, the first three elementary reactions, except R38, promoted the temperature rise of C_2H_6 at various equivalence ratios. At $\Phi = 0.8$, the order is R99 OH + CO <=> H + CO_2, R119 HO_2 + CH_3 <=> OH + CH_3O. When the equivalence ratio is 1.0, it is R99 OH + CO <=> H + CO_2, R74 H + C_2H_4 (+M) <=> C_2H_5(+M). At $\Phi = 1.2$, it is R119 HO_2 + CH_3 <=> OH + CH_3O, R166 HCO + H_2O <=> H + CO + H_2O.

For the first three important elementary reactions to inhibit the temperature rise of C_2H_6, when the combustion is under lean condition, the reactions are R159 $2CH_3$ <=> H + C_2H_5, R35 H + O_2 + H_2O <=> HO_2 + H_2O and R52 H + CH_3(+M) <=> CH_4(+M). At the stoichiometry, they are also R159, R52 and R35, but the sensitivity coefficients changes. At $\Phi = 1.2$, the order is R52 H + CH_3(+M) <=> CH_4(+M), R55 H + HCO <=> H_2 + CO and R158 $2CH_3$(+M) <=> C_2H_6(+M). It is noteworthy that R52 suppress temperature rise during rich combustion of C_2H_6. In lean combustion and stoichiometric ratio, R159 produces active H, which leads to the increase of H concentration in premixed combustion of C_2H_6, thus promoting the overall chemical reaction rate. Maybe this is one of the reasons why the LBV of C_2H_6 is faster than methane.

By comparing the blending of FH_2, it is seen that the temperature sensitivity of R38 increases when the hydrogen ratio is 40% in lean and stoichiometric conditions, but decreases for

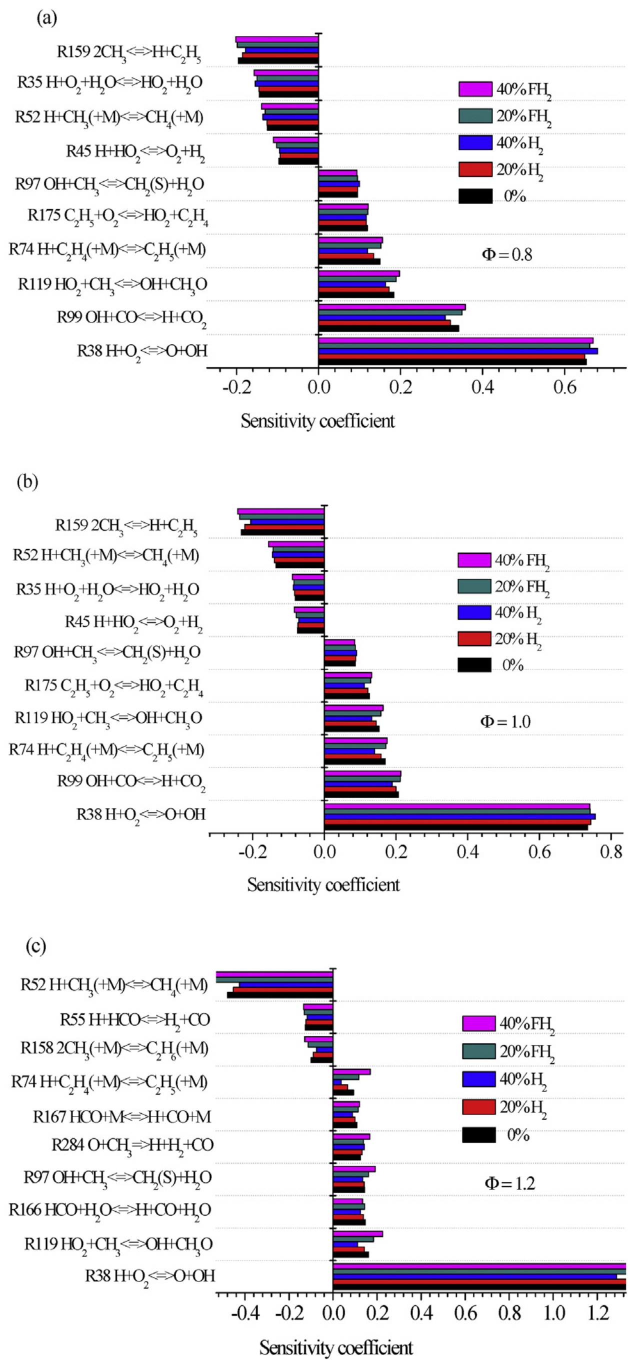

Fig. 11 – Sensitivity coefficients of C_2H_6 temperature with H_2 and FH_2 addition at different equivalence ratios.

other important elementary reactions. For the same equivalence ratio and hydrogen doping ratio, in addition to R97 in lean and stoichiometric conditions, the addition of FH_2 increases the sensitivity of the elementary reaction that plays a vital role in the temperature change of C_2H_6.

Conclusions

Using the premixed free-propagating flame model based on Chemkin II/Premix Code, the influence of H_2 addition on the combustion characteristics of laminar premixed flame of methane and ethane was systematically studied. Firstly, the effects of different initial temperatures (298–473 K) and pressures (1–5 atm) on LBVs and AFTs of methane and ethane in the equivalence ratio range of 0.5–1.6 were compared and analyzed. Subsequently, the physical and chemical effects of H_2 on LBVs, AFTs, NHRRs and the responsible elementary reactions on temperature rise of methane and ethane laminar premixed flames were discussed under lean ($\Phi = 0.8$), stoichiometric ($\Phi = 1.0$) and rich ($\Phi = 1.2$) conditions at different hydrogen doping ratios (0–40%). The major conclusions are summarized as follows.

(1) At the same pressure, the LBV and AFT increase with increasing initial temperature. The equivalence ratio of the maximum LBV of CH_4 at different initial temperatures is 1.05, while that of C_2H_6 is 1.10. Different from LBV, the equivalence ratios of maximum AFTs of methane and ethane are 1.05, only the equivalence ratios of maximum AFT and LBV of C_2H_6 are different.
(2) The LBVs of the two fuels decrease with the increase of pressures at the identical temperature. The higher the initial temperature is, the more obvious the effect of pressure on the decrease of LBV is, and the decreasing LBV of CH_4 is the largest when the pressure increases. At the same temperature, the pressure increases from 1 to 5 atm, and the LBV of CH_4 decreases to 1/2 of the original, while C_2H_6 decreases to about 1/3.
(3) The effect of hydrogen addition on the LBV of CH_4 in the rich combustion zone is greater than that in the lean. The LBVs of CH_4 and C_2H_6 is greatly increased by hydrogen addition, and enhanced by the chemical effect of H_2. The LBV decreases with the physical effect of H_2. The chemical effect of H_2 is twice that of physical effect, so the overall effect of hydrogen doping is to increase the LBV. The effect of H_2 decreases with the increase of carbon atom number of alkanes. The physical and chemical effects of H_2 on the AFT are similar to that of LBV. The difference is that the H_2 addition has slight influence on the changes of AFT.
(4) The NHRRs of methane and ethane increases with the increasing of hydrogen doping ratio. However, the flame temperature corresponding to the peak of NHRR decreases with the hydrogen doping ratios increase. Compared with FH_2, the physical effect of H_2 inhibits the combustion chemical reaction, leading to the decrease of NHRR. The chemical effect of H_2 accelerates the process of chemical reaction and obviously improves the NHRR of laminar premixed combustion.
(5) The two most critical elementary reactions for promoting the temperature rise of methane and ethane are $H + O_2 <=> OH + O$ and $CO + OH <=> H + CO_2$. The important reactions responsible for inhibiting the temperature rise are $H + CH_3(+M) <=> CH_4(+M)$ and $H + O_2 + H_2O <=> HO_2 + H_2O$.

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