Simulation of laminar burning velocity of Methane/Hydrogen/Air premixed mixtures

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Abstract

The laminar burning velocities of hydrogen-air and hydrogen-methane-air mixtures are very important in designing and predicting the process of combustion and performance of combustion systems where hydrogen is used as fuel. In this study laminar burning velocities of hydrogen-air and different compositions of hydrogen methane air mixtures (from 100% methane to 100% hydrogen) have been predicted using Chemkin, Premix code employing GRI-Mech 3.0 reaction mechanism for methane oxidation at ambient temperature for variable equivalence ratios (Φ=0.5-1.5). The results show that increasing the hydrogen percentage in the hydrogen-methane mixture increases the burning velocity which is consistent with the published experimental data.

Keywords: Burning velocity; Hydrogen-Methane mixture; Chemkin

1-Introduction:

Natural gas, which is mainly composed of methane, offers significant economical and environmental advantages over other fuels [1]. Hydrogen–methane blends are receiving attention as alternative fuels for power generation applications for two main reasons. The first reason is related to the opportunity of adding Hydrogen to methane in order to improve performance, to extend operability ranges and to reduce pollutant emissions of lean combustion in both stationary and mobile systems. The second reason is due to concerns about global warming and the prospect of using hydrogen in both, fuel cells and combustion devices. However, stringent problems of safety and storage strongly complicate the use of pure hydrogen. To bypass these difficulties, substitution of hydrogen with methane or other hydrocarbons has been proposed as an interim solution towards a fully developed hydrogen economy [2].

Laminar burning velocities of methane-air mixtures as a function of temperature, pressure and equivalence ratio have been measured by many investigators using several experimental techniques. The experimentally determined laminar burning velocity results were inconsistent for a long time [3]. The laminar burning velocity for a stoichiometric mixture at ambient conditions varied typically between 35 and 45 cm/s [4].

The laminar burning velocity of hydrogen–methane/air premixed flames has been experimentally measured at different values of equivalence ratio and fuel composition. Scholte and Vaags [5] carried out the first measurements by means of the tube burner method which is the most extensive experimental study since it investigates a wide range of equivalence ratios at hybrid fuel compositions varying from pure methane to pure hydrogen. All the other experimental papers may be classified into two categories [2]. The first deals with the study of the effect of hydrogen addition to methane and the second with the effect of substitution of hydrogen by methane. According to these results when hydrogen is added to methane, a linear increase of the laminar burning velocity occurs with increasing the hydrogen mole fraction in the fuel (X_{H_2}) up to values equal to about 0.7. Furthermore, the enhancement is slight, especially at lower equivalence ratios. On the contrary, at high hydrogen molar contents (X_{H_2} >0.85), the burning velocity rate is increased sharper than the other regimes [2].

Experimental results of hydrogen burning velocity of other authors are also available in the present study where for example the maximum laminar burning velocity at ambient conditions ranges from 260 to 350 cm/s [4].

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2-Model

A freely propagating, adiabatic, premixed, planar flame was simulated with PREMIX, sandia's steady-state, laminar, one-dimensional flame code. PREMIX uses a hybrid time-integrating/Newton iteration technique to solve the steady-state mass, species and energy conservation equations and can be set up to simulate a premixed propagating flame. The systems of equations are solved using TWOPNT, a boundary value problem solver in the CHEMKIN II package [6]. An additional boundary condition for mass flow rate, which is necessary for this type of formulation, was obtained by fixing the location of the flame by specifying the temperature at one point. The CHEMKIN package [6] was modified to implement the GRI mechanism by replacing its original reaction and transport library with the GRI files. In this study, the GRI mechanism version 3.0 [7] , which has 325 reactions and 53 species, was used without any modification. The mechanism is described extensively elsewhere [1, 8].

The problem environment was defined by setting the initial and boundary conditions. The initial flow rate estimation of the fuel/oxidizer mixture was set equal to 0.04 (g/cm^2 .s) according to the published measurements of stoichiometric methane/air burning velocity [2]. The pressure and temperature of the mixture were set at 1.0 atm. and 298 K, respectively. The additional boundary condition required for the flow solution was supplied by fixing the temperature point for 400 K whose distance is calculated from the initial temperature profile estimation by the software. Since it was known from the previous studies that the total reaction zone of the premixed, laminar, freely propagating, stoichiometric methane/air flame is about 0.4 cm, the calculation domain was started 2 cm before the flame region and the total length of the calculation domain was chosen as 12 cm[2]. The initial temperature profile estimation, which is required to start the iteration, was made according to the recent study of VanMaaren et al [9]. Results of the first simulation step were used as the temperature profile estimation for the next step [1].

3-Results and Discussion

3-1- Pure methane and pure hydrogen burning velocity

The solution algorithm was first tested for accuracy by comparing the burning velocity at different equivalence ratios and ambient condition of pure methane/air and pure hydrogen/air mixtures to published values [1].Fig.1 illustrates the good agreement between the simulation and experimental results. The experimental results were done by different publishers [3, 4]. The burning velocities of methane-air mixture were also predicted by H.M.Heravi [10] employing GRI-Mech 2.11 [11] are shown in this Fig.
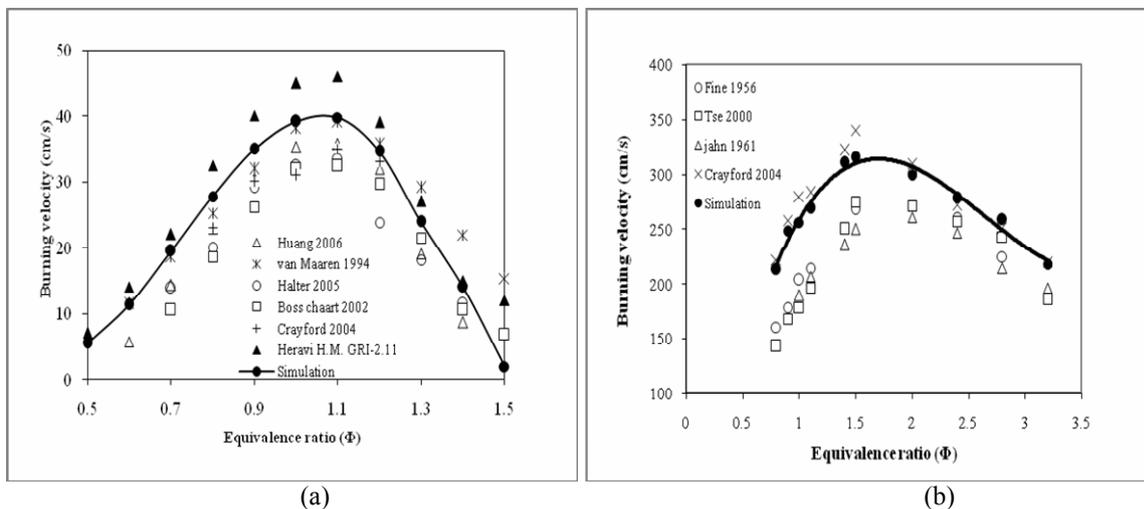

|(a)|(b)|

Fig 1.Pure methane burning velocity simulation result in compare with experimental data (a)
Pure hydrogen burning velocity simulation result in compare with experimental data (b)

Further more in this article evaluating the burning velocity at different pressures is done. A good prediction is obtained in all the regimes at lean, stoichiometric and rich mixtures at NTP (normal temperature and pressure) conditions. This agreement is also found for the computational results of mixtures at higher than normal values of initial pressure (up to 10 atm.) [2, 12].

Fig.2 shows the simulated results for methane/air mixture burning velocity at different pressures. Calculated data clarify that increasing the pressure causes the burning velocity to be reduced.
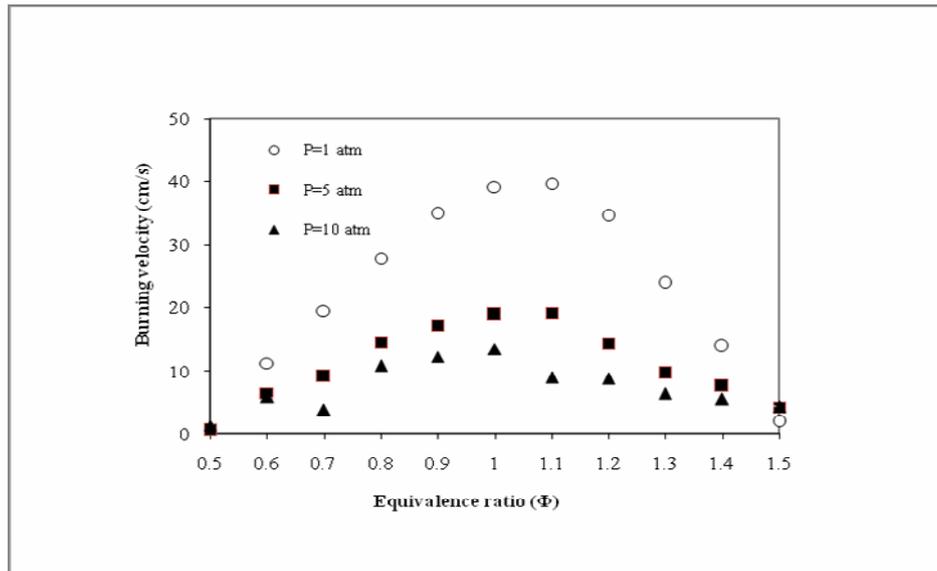
Fig.2 Burning velocity at different pressures

3-2- Methane/hydrogen/air laminar burning velocity Predictions

The laminar burning velocities of hydrogen–methane/air mixtures at 300K and 1 atm were calculated by varying the equivalence ratio from lean to rich conditions and the fuel composition from pure methane to pure hydrogen. In Fig. 3 the computed values and experimental results [3] are plotted versus the hydrogen mole fraction in the fuel (X_{H_2}), at stoichiometric condition. From Fig.3, at all the equivalence ratios, it is possible to identify three regimes in the hybrid flame propagation depending on the hydrogen mole fraction in the fuel.

At low hydrogen contents $(0< X_{H_2} <0.5)$, a regime of methane-dominated combustion takes place being characterized by a linear and slight increase of the methane laminar burning velocity on adding hydrogen.
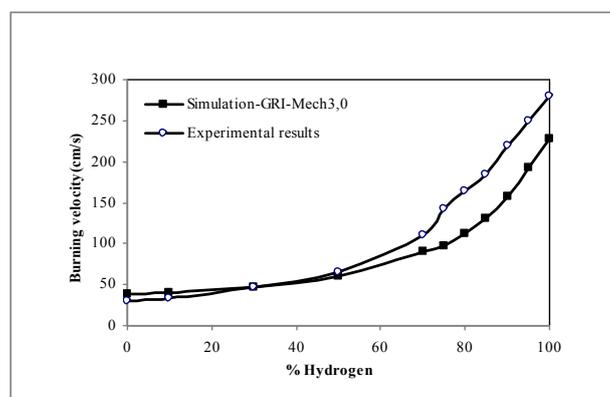

Fig.3 Comparison of experimental and computational results of hydrogen addition to methane on burning velocity at Φ=1

At high hydrogen contents $(0.9< X_{H_2} <1)$, a regime of methane-inhibited hydrogen combustion occurs corresponding to a linear and sharp decrease of the hydrogen laminar burning velocity on increasing the methane presence in the fuel. At intermediate hydrogen mole fractions $(0.5< X_{H_2} <0.9)$, a transition regime is found. It appears that at lean and stoichiometric conditions a good prediction is obtained. This applies also to the rich mixtures with low hydrogen contents $(X_{H_2} <0.7)$.

3-3- Effect of hydrogen addition on the pollutant concentration

Pollutant concentrations play one of the most important roles in combustion systems due to global warming, health care and devastative effects on the environment. Therefore the pollutant concentration and it's relation

with the temperature profile is discussed in this paper. Temperature profiles of different mixtures for the whole flame area are illustrated in Fig. 4.
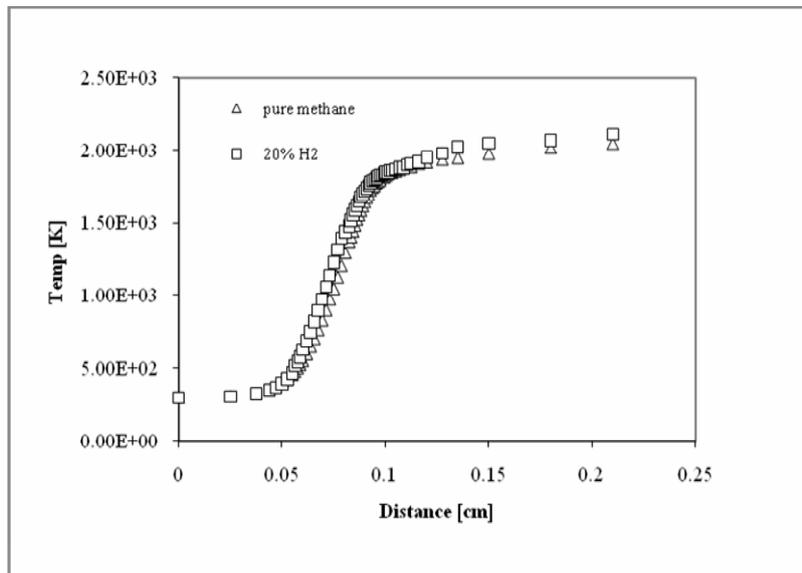

Fig 4.Temperature profile for pure methane and methane/hydrogen/air flame

Although all mixtures appear to have similar temperatures profile, But Hydrogen has a higher flame temperature in compare with methane, and the flame temperature of the mixture was increased by less than 1% even with the addition of 20% H_2. However the temperature is increasing by addition of H_2 to CH_4 but the addition of hydrogen causes the overall carbon to hydrogen ratio of the mixture to decrease (a pure hydrogen flame produces no CO). As a result, CO concentrations for the hydrogen added mixtures were decreased. Differences in CO concentrations for all lean mixtures were negligibly small, due to the low CO concentration found at these equivalence ratios [1].Fig.5-a illustrates the pollutant concentrations versus equivalence ratio. The effects of hydrogen addition on NO concentrations for different equivalence ratios in methane/air mixtures are shown in Fig.5-b.
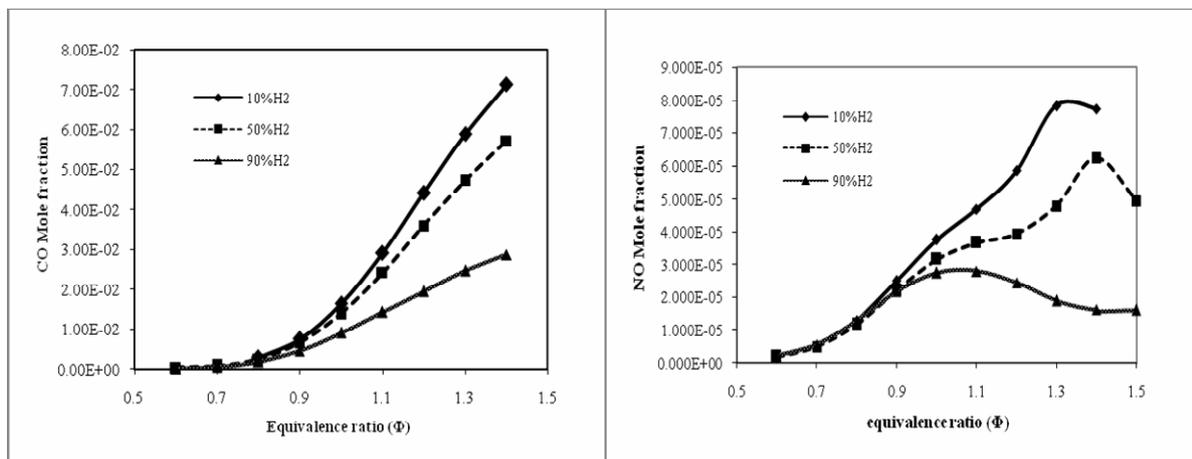
(a)   (b)

Fig5. Concentration of CO and NO as a function of equivalence ratio a) CO , b) NO

With hydrogen/methane mixtures, the slight increase in temperature due to addition of H_2 is compensated by the decrease in oxygen concentration, leading to lower NO concentrations in lean mixtures. However, for lean mixtures, differences in NO emissions are very small.

4- Flame thickness

A typical flame temperature and fuel concentration profile from the results of Chemkin, Premix is shown in Fig.6. The flame structure generally consists of two regions, referred to as preheat and reaction zone [9].It is not easy to distinguish the inflexion point where the preheat zone ends and reaction zone starts. However, consistent with and corresponding to the shape of the temperature profile at its maximum slope dT/dX that corresponds to the segment of the tangent spanning the temperature interval between unburned gas temperature (T_u) and burned gas temperature (T_b) is generally taken as a measurement for the flame thickness, that is X, Fig. 6.
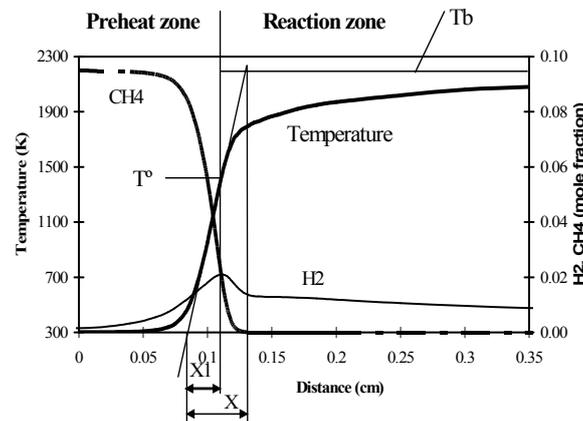

Fig.6 Measurement of flame thickness from the temperature profile [10].

Fig 7.shows the comparison of predicted flame thickness obtained by H.M.Heravi [10] with GRI-Mech 2.11 [11], experimental data of Andrews and Bradley [13] and the present results of simulation with GRI-Mech 3.0 [ ] for pure methane oxidation, also pure hydrogen and the mixture of 60% H_2+40%CH_4. The measurement of Andrew & Bradley [13] using thermocouples and schieldern photography are higher than that of others over the whole range. Possibly this arises from the difficulties in measuring the flame thickness directly due to the nature of the thin flame and difficulties in compensating the fine thermocouples for the effect of frequency response, radiation and other losses[10].
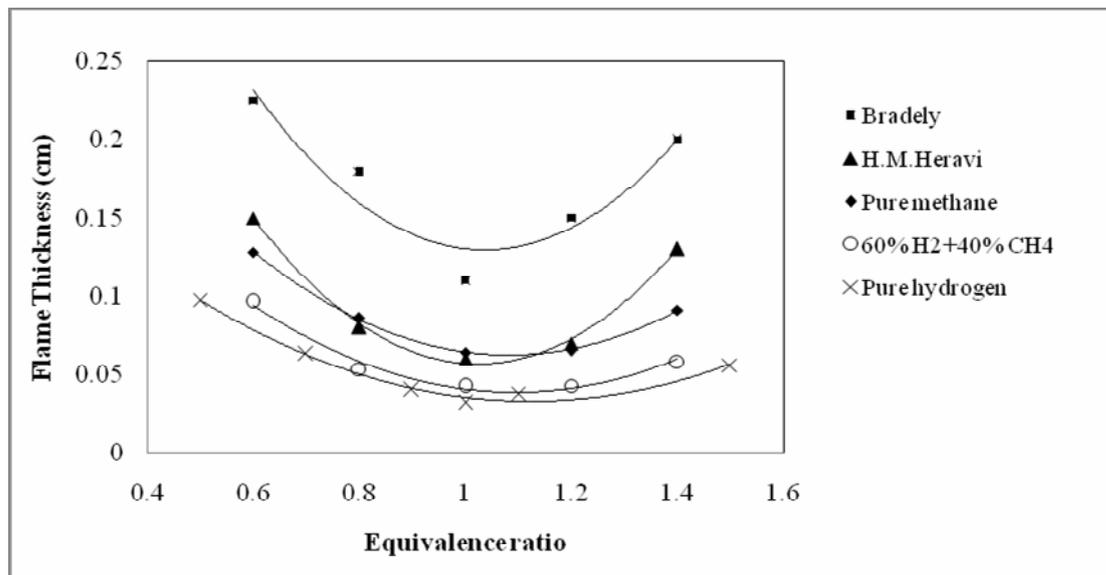

Fig.7 flame thickness versus equivalence ratio

In Fig.8 both the flame thickness and burning velocity for the methane-hydrogen-air mixture at stoichiometric condition with varying the hydrogen percentage in fuel from 0% to 100% are shown. It can be seen that as the hydrogen content in fuel increased the flame thickness is decreased but the burning velocity is increased.
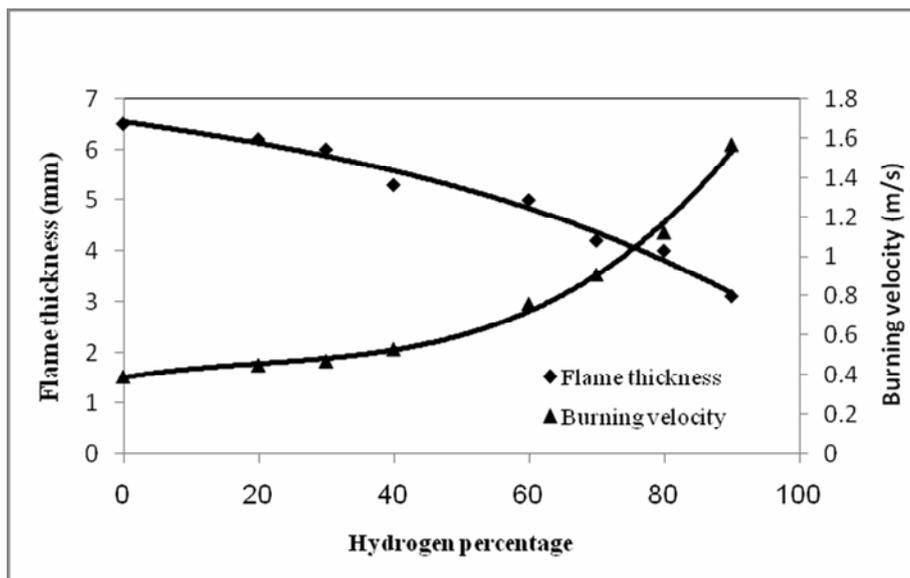
Fig.8 Flame thickness and burning velocity

5-Conclusion

- The laminar burning velocities of methane-hydrogen-air premixed flames are predicted by means of Chemkin Premix Code implementing the GRI-Mech 3.0 detailed reaction mechanism are in good agreement with the published experimental data.
- As the percentage of hydrogen is increased in the methane-hydrogen air mixture, the burning velocity increases, but the flame thickness decreases.
- The effect of pressure on burning velocity has been studied and the results show that as the pressure is increased the burning velocity is decreased.
- Both CO and NO_x concentrations are decreased by increasing the hydrogen percentage on the methane-hydrogen-air mixture.

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