THE ADIABATIC FLAME TEMPERATURE AND LAMINAR FLAME SPEED OF METHANE PREMIXED FLAMES AT VARYING PRESSURES

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This paper studies the influence of equivalence ratio, pressure and initial temperature on adiabatic flame temperature and laminar flame speed of methane-air mixture. The results indicate that adiabatic flame temperature is weakly correlated with pressure. The adiabatic flame temperature increases only by about 50 ℃ as a result of 30 bar pressure increase. The flame speed is inversely proportional to pressure. The maximum adiabatic flame temperature and flame speed occur at the stoichiometric ratio, Φ=1. The percent increase in the flame speed was about 400% when the initial temperature of the mixture is increased from 25 ℃ to 425 ℃.

INTRODUCTION

Flame propagation plays a primary role in the design and optimization of many combustion applications. In general applications, from domestic appliances to engines and gas turbines, pressure and initial temperature of the mixture are often higher than standard ones. Analytical correlations of the laminar flame speeds and adiabatic flame temperature as a function of equivalence ratio, pressure and temperature are preferred in practical simulations. In the last decades, various forms of empirical and semi-empirical functional relationships have been proposed for the laminar burning velocity (1, 2).

Experimental and simulation was implemented in the last few years to study the flame speed and adiabatic flame temperature of several fuels and fuel mixtures, for instance, S.Hu et al. (3) studied Laminar methane/air premixed flames at different pressures in a newly developed high-pressure Bunsen flame rig using detailed numerical simulations and laser diagnostics. Stephen W.Grib and Michael W.Renfro (4) studied Triple (or tribrachial) flames propagation using a laminar five slot burner, which allows both the concentration gradients and stoichiometric separation distance of two interacting triple flames to be varied. B. Zhang et al. (5) studied the laminar flame speed of natural gas/carbon monoxide fuel mixtures by experimental and numerical methods. Experimental measurement shows that with the increase of the volume fraction of natural gas, the maximum laminar flame speed of natural gas/carbon monoxide fuel blend first increases and then decreases, and the peak value is obtained at 0.748 m/s for 8% natural gas in the fuel blend. C. Dong et al. (6) studied the Laminar Flame Speed of Hydrogen, Carbon Monoxide, and Natural Gas Mixtures with Air, the measured laminar flame speeds of hydrogen/carbon monoxide/natural gas/air mixtures (at lean and rich conditions) show an increasing trend with volumetric fraction of hydrogen or carbon monoxide and a decreasing trend with volumetric fraction of natural gas. Hasan Kayadelen (7) introduced a new multi-featured equilibrium combustion model for fuels, fuel blends, and surrogates which estimates mole fractions, adiabatic flame temperature and thermodynamic properties of the equilibrium combustion products. Siyuan Hu et al. (8) conducted a numerical and experimental study on laminar methane/air premixed flames at varying pressure. In their

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work, the methods of flame-cone-angle and flame-area have been used to extract the laminar flame speed for different equivalence ratios and pressures. Akram Mohammad and Khalid A. Juhany (9) studied the influence of mixture equivalence ratios, blend combinations, and initial temperatures on laminar burning velocity and flame structure of DME/methane+air mixtures at elevated temperatures. They found that the rate of increase in burning velocity with respect to an increase in initial temperature is higher for pure methane+air mixtures. Mahdi Faghih et al. (10) studied laminar flame speed from low-pressure and super-adiabatic propagating spherical flames. They used numerical simulations considering detailed chemistry and transport to study spherical flame propagation at low pressures or with super-adiabatic flame temperature.

Jamil J. Al Asfar et al. (11), simulated a two-dimensional (2-D) modeling of the burning process of Jordanian oil shale in a circulating fluidized bed (CFB) burner. It was found that the temperature contours of the combustion process showed that the adiabatic flame temperature was 1080 K in a vertical burner.

Certain applications like industrial gas turbines require pressures as high as 30 atm and operate at temperatures close to minimum ignition temperature. It is therefore important to quantify the effects of pressure and initial temperature on the adiabatic laminar burning velocity of many practical fuels. This work used numerical simulations considering detailed chemistry to study the adiabatic flame temperature and laminar flame speed of methane premixed flames at varying pressures. The calculated results are in agreement with published experimental results.

RESULTS AND DISCUSSION
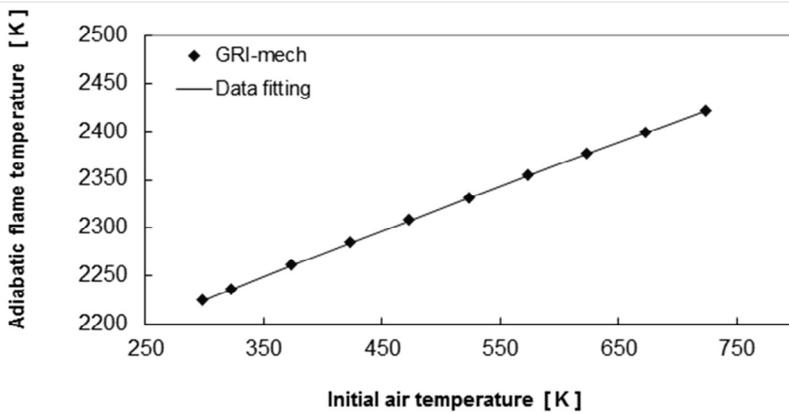
Flame temperature

Flame temperature is one of the most important properties in combustion since it has a controlling effect on the rate of a chemical reaction. The flame temperature is determined by the energy balance between the reactants and the products at equilibrium. If the reaction zone is spatially very thin in comparison to the rest of the domain of interest, then it is a common practice to denote the maximum temperature in the reaction zone to be the flame temperature. If the combustion process takes place adiabatically, with no work, or changes in the kinetic or potential energy, then the flame temperature is referred to as the adiabatic flame temperature. This is the maximum temperature that can be achieved for the given reactants because any heat transfer from the reaction zone and any incomplete combustion would tend to lower the temperature of the products.

The factors of prime importance to adiabatic flame temperature are fuel-air ratio, initial air temperature, pressure, and fuel type. The adiabatic flame temperature is a strong function of the relative air-fuel ratio wherever it reaches a maximum value slightly beside the stoichiometric due to dissociation effects. While in the lean region excess air is supplied to the system resulting in an increase in the heat loss from the flame, in the rich region insufficient air is supplied leading to incomplete combustion and also to flame temperature decrease. CHEMKIN was used to illustrate the variation of the adiabatic flame temperature with air-fuel ratio (λ). The obtained results for methane at ambient pressure and temperature are shown in Figure 1 and correlated using Eq. 1. The adiabatic flame temperature was simulated using CHEMKIN with changing the initial temperature of the mixture and holding both pressure and air-fuel ratio constant. The results are presented in figure 2 and correlated using Eq. 2.
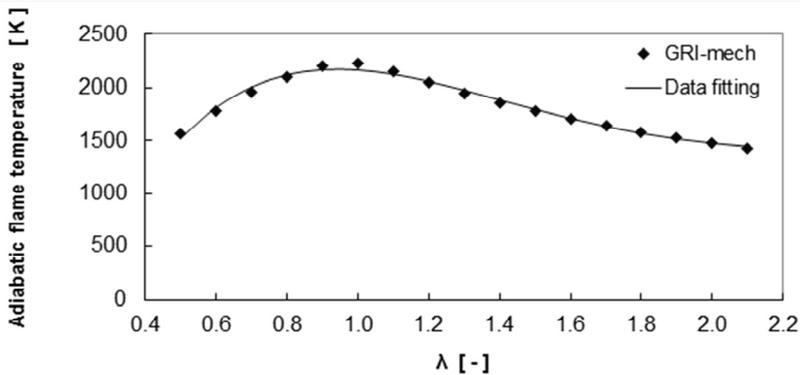
Figure 1. Air-fuel ratio dependency of the methane adiabatic flame temperature at ambient pressure and temperature (CHEMKIN calculation).

$$T_{adiab}\,(K) = Exp\left[9.1418 - \left(\frac{1.4727}{\lambda}\right) - 1.6161 * \ln \lambda\right] \qquad [1]$$

Figure 2. Initial air temperature dependency of the methane adiabatic flame temperature at atmospheric pressure and stoichiometric air-fuel ratio (CHEMKIN calculation).

$$T_{adiab}(K) = 2087.2 + 0.46502 * T_i(K) \qquad [2]$$

Flame temperature is weakly correlated with pressure. This can be clearly seen from the correlation; Eq. 3; obtained from studying the effect of pressure on the adiabatic flame temperature at stoichiometric conditions and ambient initial air temperature.

$$T_{adiab}(K) = \frac{1407.7 + 2314.2 * p(atm)^{0.39908}}{0.67297 + p(atm)^{0.39908}} \qquad [3]$$

The obtained results are shown in Figure 3, which indicates that the adiabatic flame temperature increases only by about 50 ºC as a result of 30 bar pressure increase.
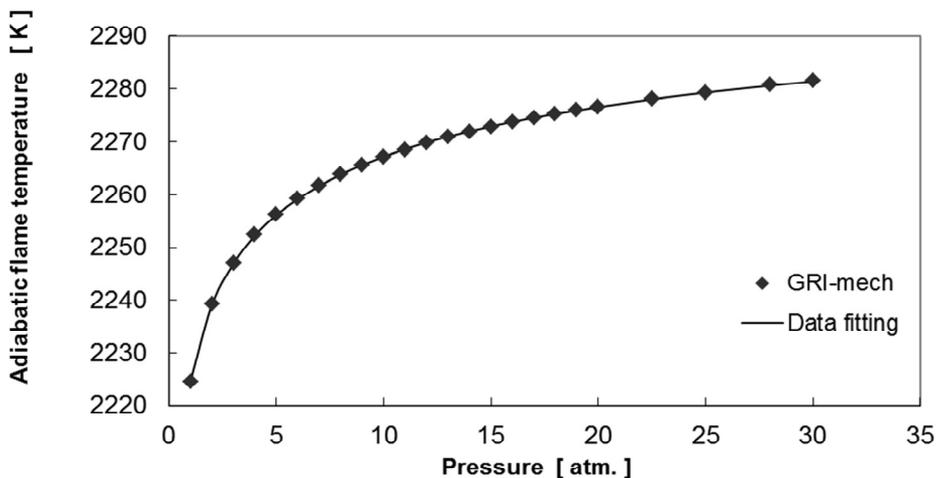
Figure 3. Pressure dependency of the methane adiabatic flame temperature at ambient temperature and stoichiometric conditions (CHEMKIN calculation).

The maximum flame temperature usually lies in the range 2200-2400 K for hydrocarbon mixtures with air and 3000-4000 K for mixtures with oxygen.
According to "laminar flame theory" (12) the flame temperature has a substantial effect on the laminar flame speed. It is widely perceived that the flame temperature essentially determines the flame speed and significantly influences the formations of the products of combustion. The concentration of oxides of nitrogen (NO_X) and carbon monoxide (CO), pollutants of great concern, are very much dependent on the flame temperature.

Laminar flame speed

The laminar flame speed which is also called the burning velocity, normal combustion velocity, or flame velocity, is more precisely defined as the velocity at which unburned gases move through the combustion wave in the direction normal to the wave surface.
Laminar flame speed is a fundamental property that is extremely useful for a number of reasons: it must be known accurately to predict the burning rate of a fuel, it is used to calibrate and validate chemical reaction mechanisms, it is needed to estimate turbulent flame speeds and it is needed to model practical turbulent premixed flames. The laminar flame speed at high pressures and temperatures is of fundamental importance for analyzing and predicting the performance of internal combustion engines and power plants.
The most important factors affecting laminar flame speed are fuel, relative air-fuel ratio, temperature, and pressure.
Many workers have investigated the effect of pressure and initial temperature on laminar flame speed. Garforth and Rallis (13) reported the measurement of the laminar

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flame speed of stoichiometric methane-air premixed flame covering dependence of both pressure and initial temperature. Toshio and Takeno (14) studied the effects of pressure and temperature on the laminar flame speed of methane-air and hydrogen-air mixtures using the spherical bomb technique. However, the pressure effects are complex. Flame theory suggests that the effect of pressure may be related to the reaction order using Eq. 4.

$$S_L \, \alpha \, p^{(n-2)/2} \qquad [4]$$

Thus, for bimolecular reaction ($n=2$) the laminar flame speed should be independent of pressure. On the other hand, experimental measurements generally show a negative laminar flame speed pressure dependency. Andrews and Bradley (15) found that the following power law; Eq. 5, can be used to correlate the laminar flame speed pressure dependency for a stoichiometric methane-air mixture for pressure greater than 5 bars.

$$S_L \, (cm/\sec) = 43 \left[p \, (atm) \right]^{-0.5} \qquad [5]$$

In agreement with experimental measurements [8] where the laminar flame speed was obtained by processing DNS, the simulation using CHEMKIN, presented in Figure 4, show that the flame speed is inversely proportional to pressure. The following shifted power formula; eq. 6; was found to correlate the simulated flame speed pressure dependency at ambient temperature and stoichiometric air-fuel ratio.

$$S_L \, (cm/\sec) = 48.128 * \left[p \, (atm) + 0.7912 \right]^{-0.51394} \qquad [6]$$
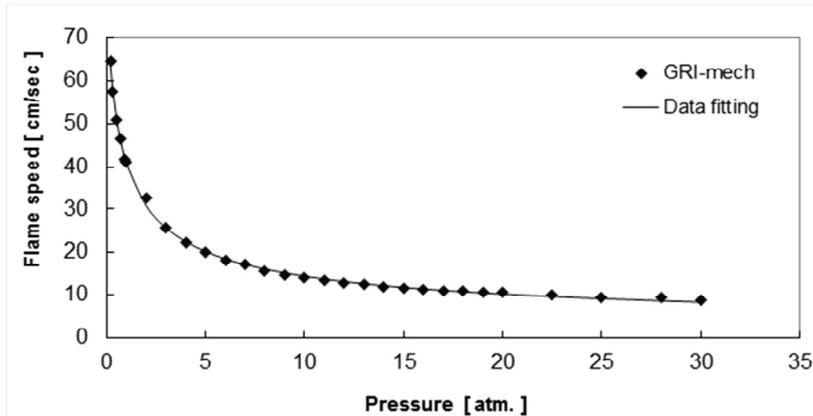
Figure 4. Methane flame speed pressure dependency at ambient temperature and stoichiometric air-fuel ratio (CHEMKIN calculation)

Figure 4 shows that the pressure has a considerable effect on the flame speed for pressures below 3 bar. Then the effect is reduced with increasing pressure. The same behavior was also obtained by Egerton and Lefebvre (16) who studied the flame speed of propane-air mixtures under pressure.

The theoretical approaches used to study laminar flame speed in premixed gases led to a proportional correlation of the form (17):

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$$S_L \; \alpha \,(thermal\ diffusitivity*reaction\ rate)^{1/2} \qquad\qquad [7]$$

In this equation; Eq. 7; the reaction rate contains the flame temperature in the exponential term, which means small changes in flame temperature leads to significant variations in the flame speed. Therefore, an increase of the flame speed with temperature is expected.

Flame speed was simulated using CHEMKIN with changing the initial temperature of the mixture and holding both pressure and air-fuel ratio constant. The obtained results are shown in Figure 5. These results are correlated by the Hoerl Model formula; Eq. 8.

$$S_L\ (cm/\sec)=0.228*(1.0022^{T(K)})*T_i(K)^{0.79719} \qquad\qquad [8]$$
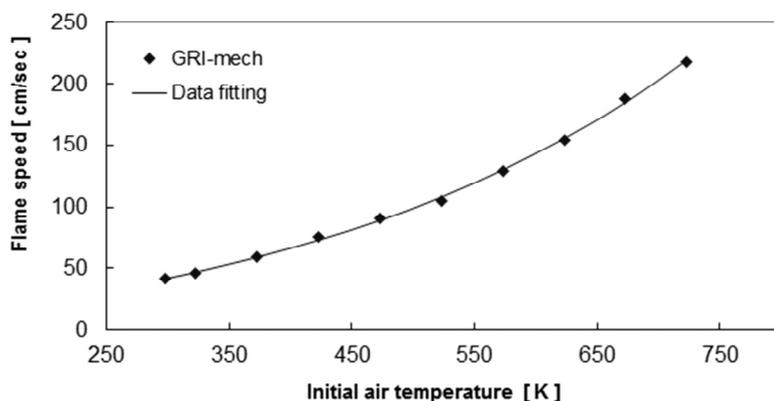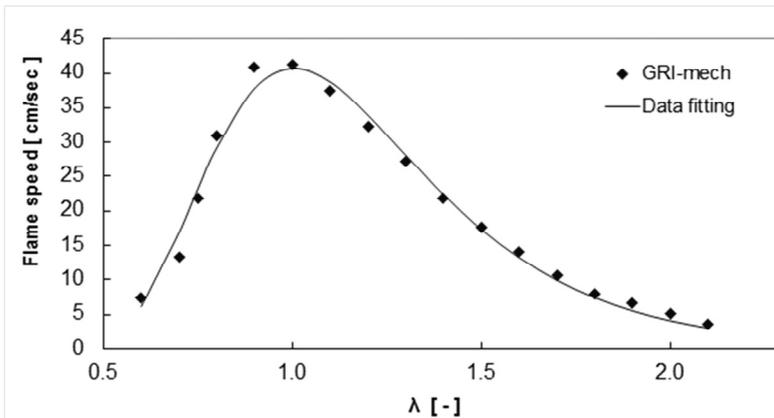

Figure 5. Methane flame speed initial air temperature dependency at atmospheric pressure and stoichiometric air-fuel ratio (CHEMKIN calculation)

The variation of the laminar flame speed with the fuel-oxidant ratio is governed predominantly by the variation of the temperature with the mixture ratio. Except for very rich mixtures, the primary effect of equivalence ratio on flame speed for similar fuels is a result of how this parameter affects flame temperatures; thus, for hydrocarbon fuels, the peak of the flame speed occurs at stoichiometric or slightly fuel rich-mixtures.

Figure 6 presents the flame speed as a function of the air-fuel ratio for methane under both ambient temperature and pressure. The simulated results are correlated with eq. 9.

$$S_L\ (cm/\sec) = Exp\left[15.739-\left(\frac{12.033}{\lambda}\right)-11.997*\ln\lambda\right] \qquad\qquad [9]$$

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Figure 6. Methane flame speed air-fuel ratio dependency under atmospheric pressure and ambient temperature (CHEMKIN calculation).

Due to complete combustion and high thermal conductivity resulted from maximum reactivity, the laminar flame speed for hydrocarbon fuels such as methane is maximum near stoichiometric conditions.

CONCLUSION

The purpose of the work is to provide simple and workable expressions for modeling the laminar flame speed and adiabatic flame temperature as a function of equivalence ratio, pressure, and initial air temperature. The flame speed is inversely proportional to pressure whereas adiabatic flame temperature is weakly correlated with pressure. A strong relation was found Methane flame speed and adiabatic flame temperature are strongly related to the air-fuel ratio of the mixture.

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