Similarities and Differences in Changes of Adiabatic Flame Temperature caused by Equivalence Ration, Pressure and Preheat between Hydrogen and Methane

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1 Introduction

The goal of this report is to investigate similarities and differences in changes of adiabatic flame temperature between popular fuel gases caused by conditions such as equivalence ratio, pressure and temperature of its mixture with air.

2 Theoretical background

2.1 Chemistry

Chemical equations of complete combustion of methane and hydrogen in air:

$$\mathrm{CH_4} + 2\,(\mathrm{O_2} + 3.76\,\mathrm{N_2}) \rightarrow \mathrm{CO_2} + 2\,\mathrm{H_2O} + 7.56\,\mathrm{N_2}$$
$$2\,\mathrm{H_2} + \mathrm{O_2} \rightarrow 2\,\mathrm{H_2O}$$

Using these equation it is possible to calculate the stoichiometric air-to-fuel ratio which is given by the formula, where m represents the mass, suffix st stands for stoichiometric conditions.

$$FAR_{st} = \frac{m_{air}^{st}}{m_{fuel}^{st}}$$

The reciprocal of the stoichiometric air-to-fuel ratio is the stoichiometric fuel-to-air ratio and is given by the formula:

$$FAR_{st} = \frac{1}{AFR_{st}}$$

Equivalence ratio formula:

$$\Phi = \frac{FAR}{FAR_{st}} = \frac{m_{fuel}/m_{air}}{(m_{fuel}/m_{air})_{st}} = \frac{n_{fuel}/n_{air}}{(n_{fuel}/n_{air})_{st}}$$

where n is representation of number of moles, suffix st stands for stoichiometric conditions

It appears form the relation above that equivilance ratios greater than one always mean there is more fuel in the fuel-air mixture than required for complete combustion (stoichiometric reaction), irrespective of the fuel and oxidizer being used.

2.2 Thermidynamics

We want to measure the temperature of flame in adiabatic combustion, in order to do that it's essential to complete the process in constant volume.

3 Description of the code

The project was done within Python 2.7 environment with Cantera implemented to it. Cantera is an open-source suite of tools for problems involving chemical kinetics, thermodynamics and transport processes. Firs of all, it was investigated what is the influence of the equivalence ratio on the adiabatic flame temperature T_a. In order to declare the proper gas the GRI-Mech 3.0 mechanism was used. Then, for 60 different values of Φ in the rage of 0.3 to 3.5, using these we could calculate temperature. The initial pressure and temperature were constant $T_0 = 300[K]$, $p_0 = 101325[Pa]$. After this we examined the influence of initial temperature on adiabatic flame temperature. For 60 different values of T in the rage form $273[K]$ to $2000[K]$ the equilibrium state was determined and temperature was calculated. During this process the initial pressure was constant and set at $101325[Pa]$. The four cases was calculated for $\Phi = [0.5, 1, 1.5, 2]$. The next step was to examine the influence of the initial pressure. We used 60 different values of pressure in the range from $0.1[atm]$ to $6[atm]$, the equilibrium state was determined and temperature was calculated. The initial temperature was constant $300[K]$. Again, the four different values $[0.5, 1, 1.5, 2]$ for Φ was used. This procedure was used for either $H2$ or $CH4$.

4 Results

4.1 Variable Φ

The Figure 1,2 presents the counted relation between the adiabatic fame temperature and the equivalence ratio of methane-air mixture and hydrogen-air mixture.

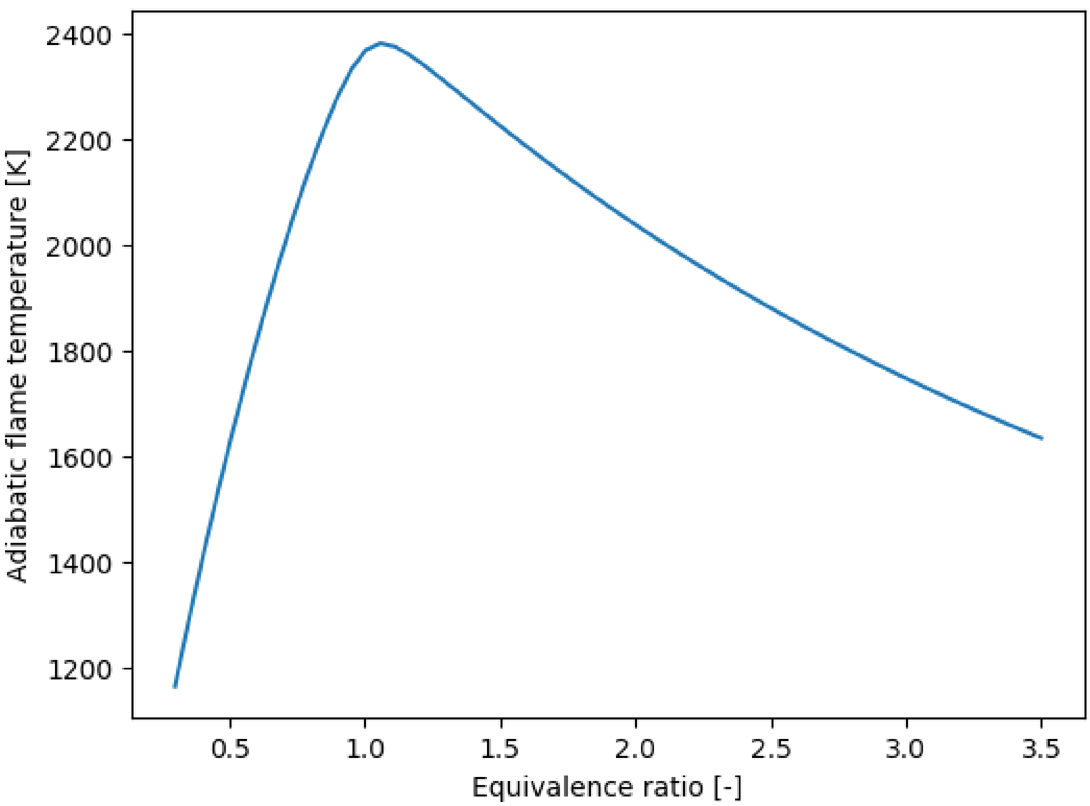

Figure 1: Hydrogen

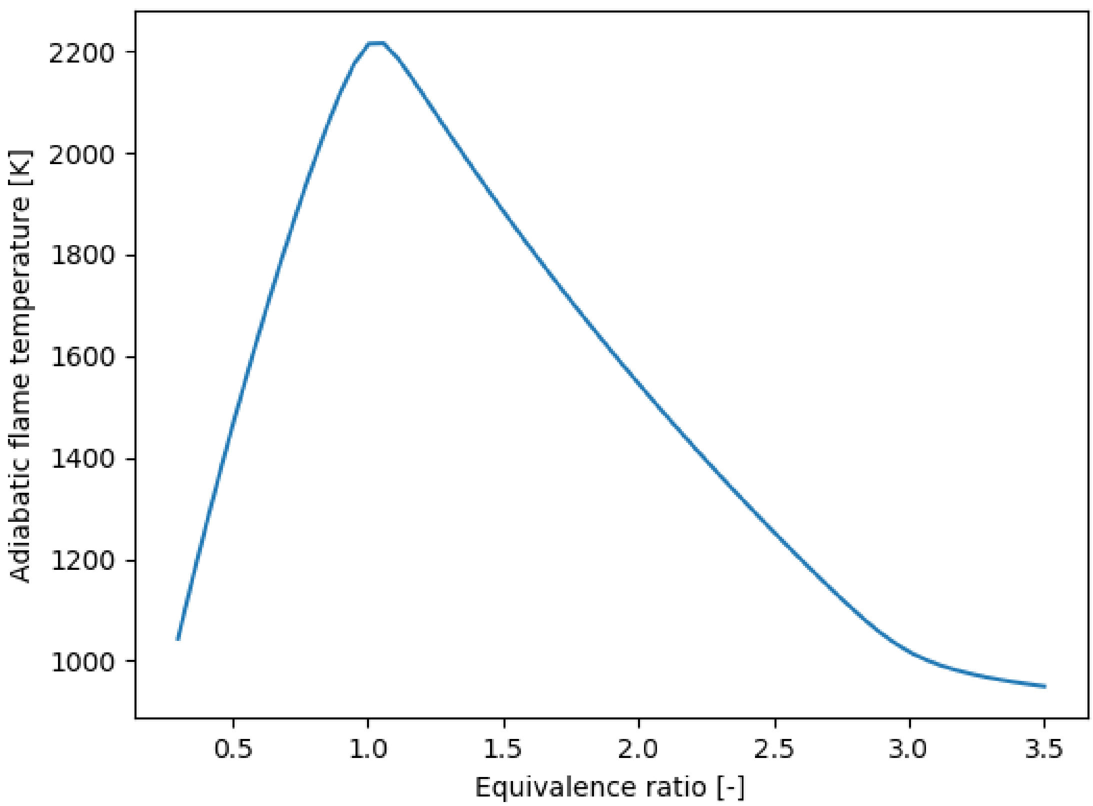

Figure 2: Methane

4.2 Variable T

Figures 3 to 12 present the counted relation between the adiabatic flame temperature and the initial value of temperature for 4 different equivalence ratios of methane-air mixture and hydrogen-air mixture. The initial pressure is $101325[Pa]$.

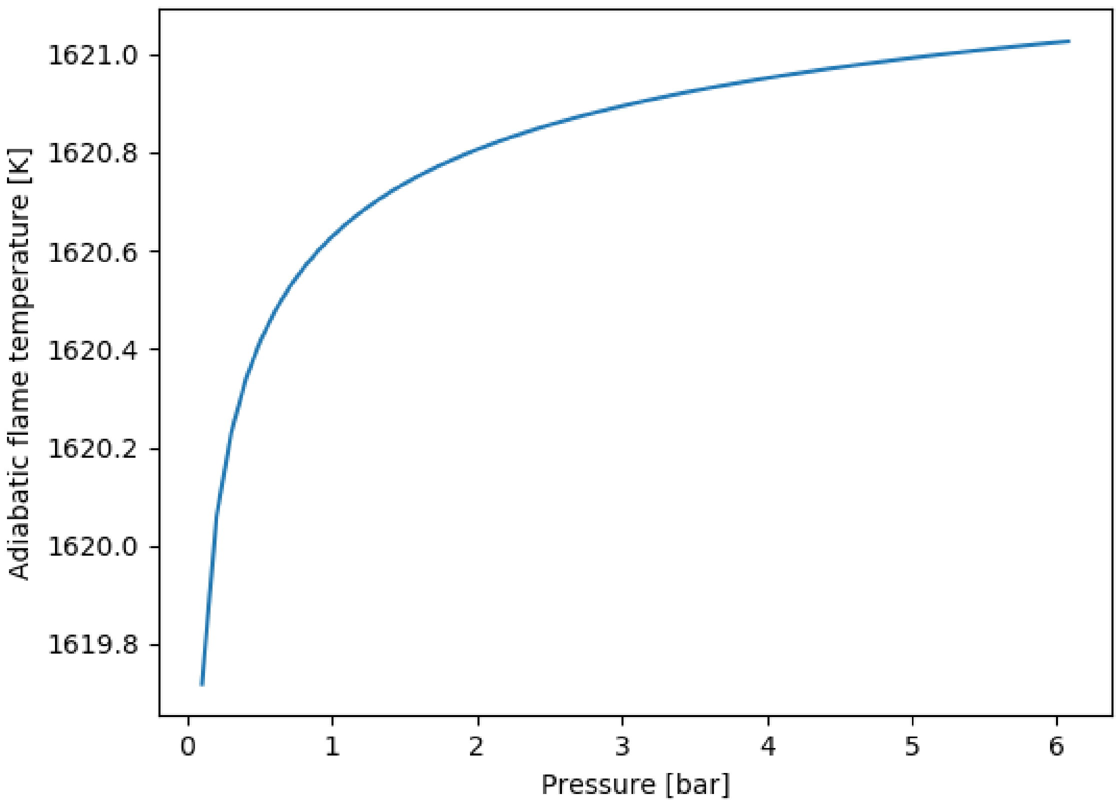

Figure 3: Hydrogen

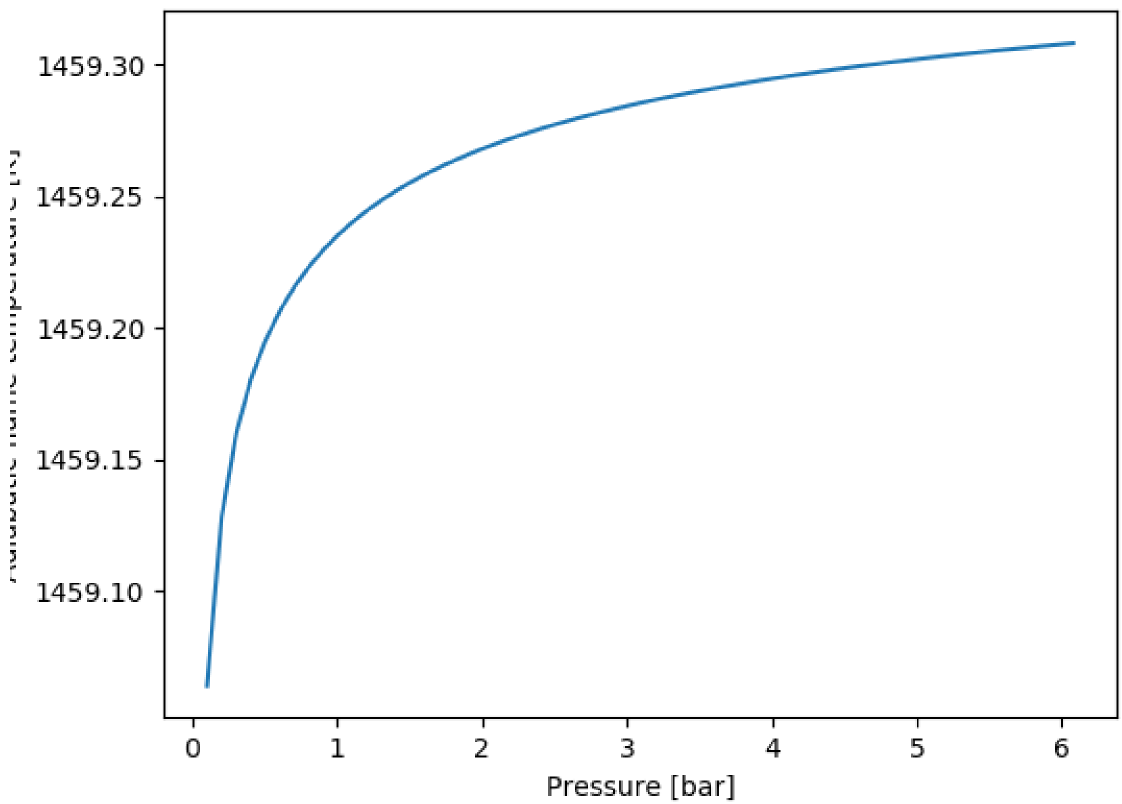

Figure 4: Methane

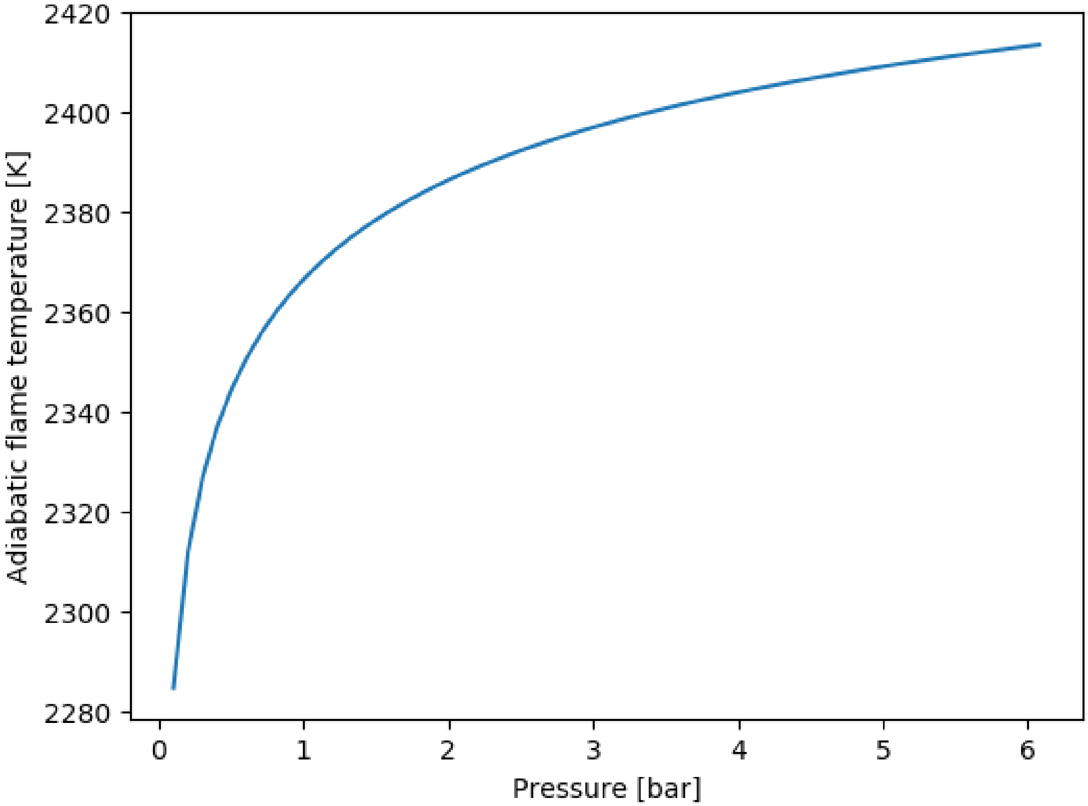

Figure 5: Hydrogen

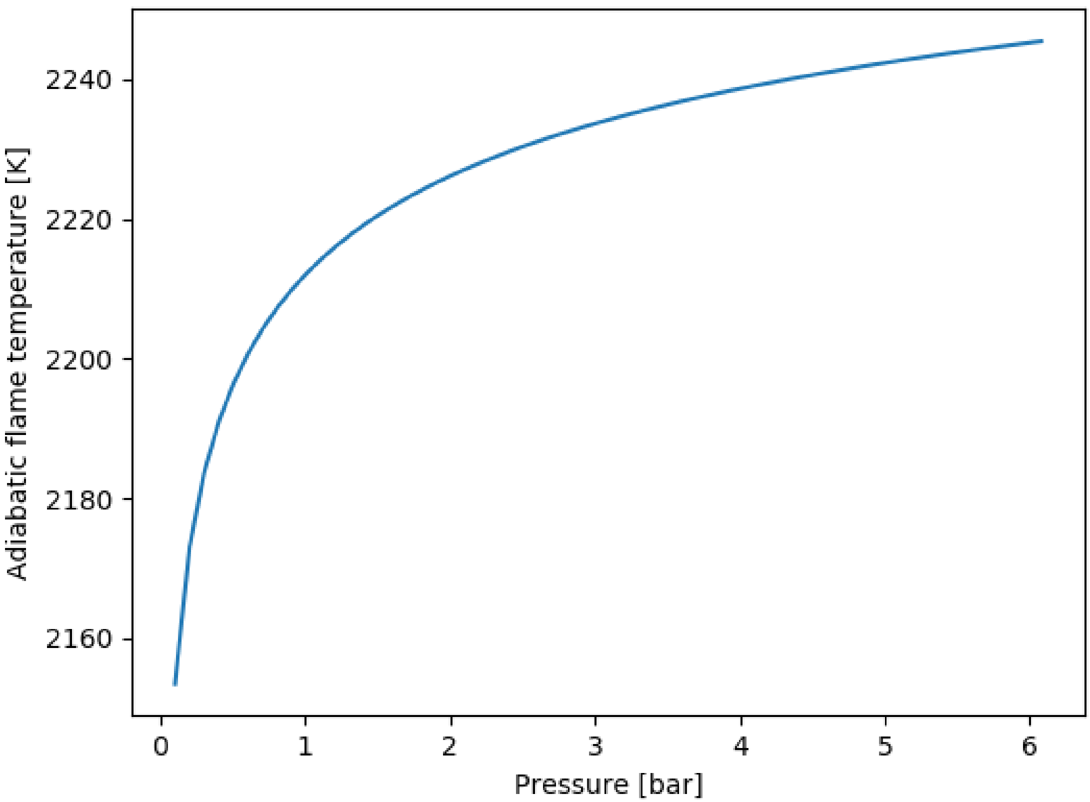

Figure 6: Methane

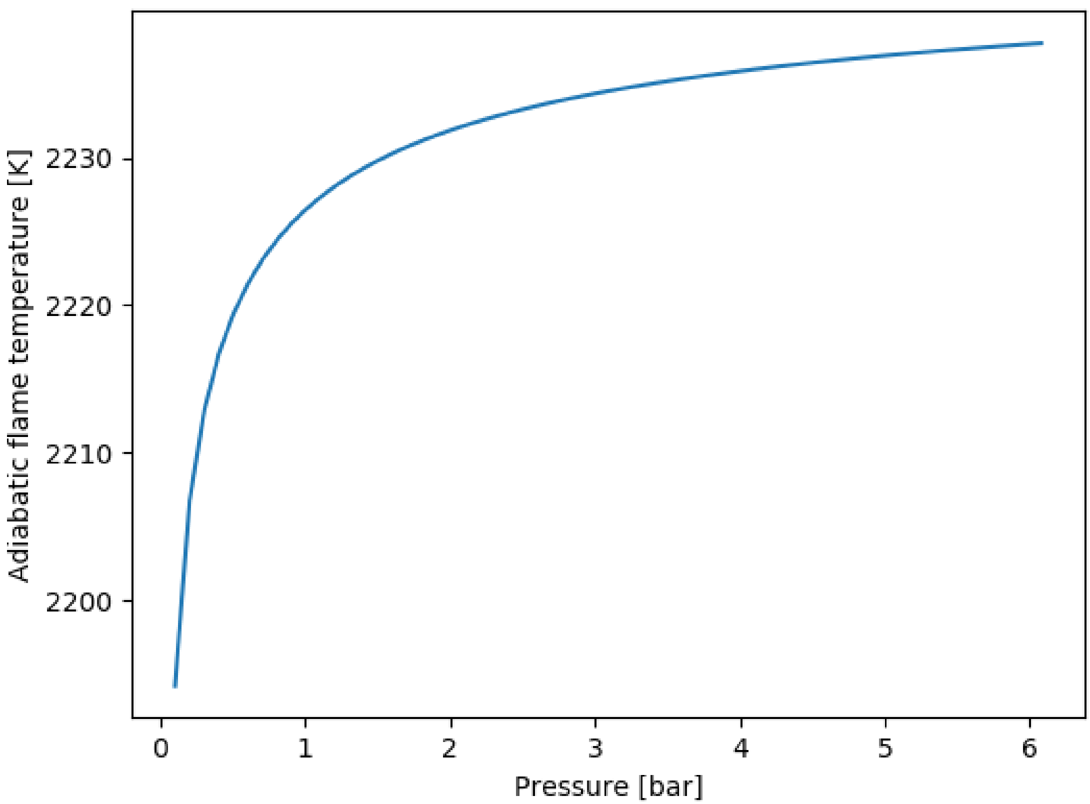

Figure 7: Hydrogen

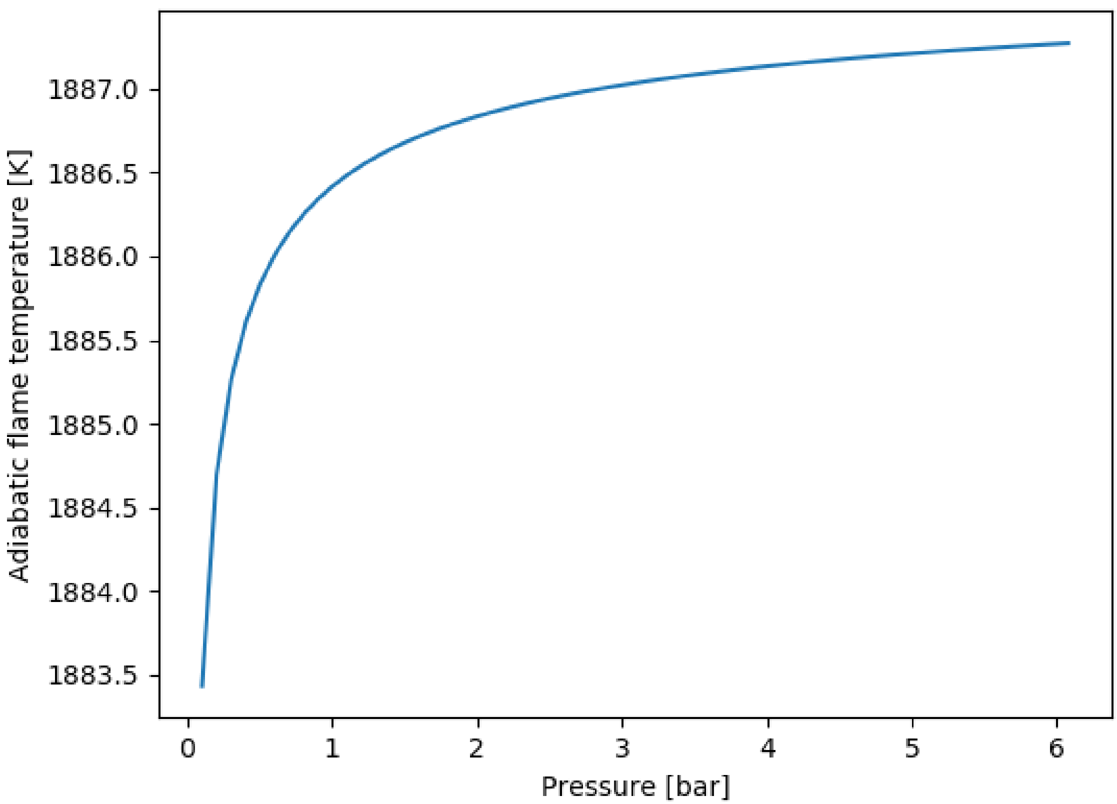

Figure 8: Methane

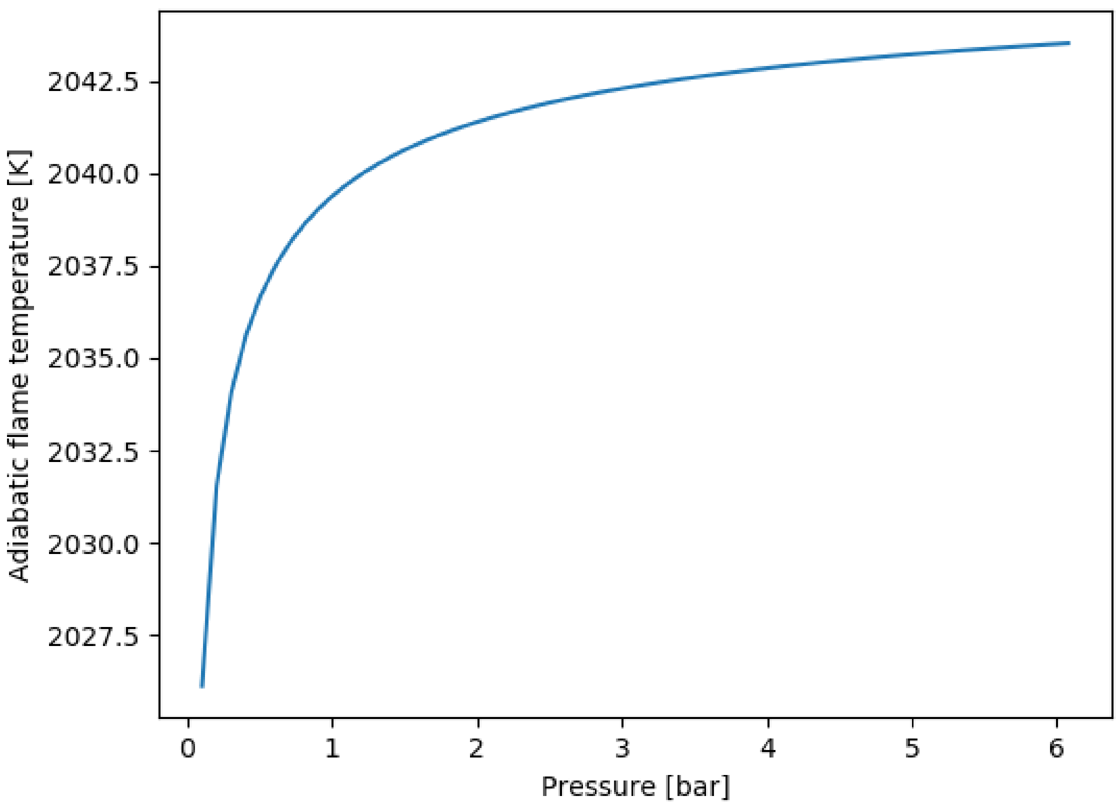

Figure 9: Hydrogen

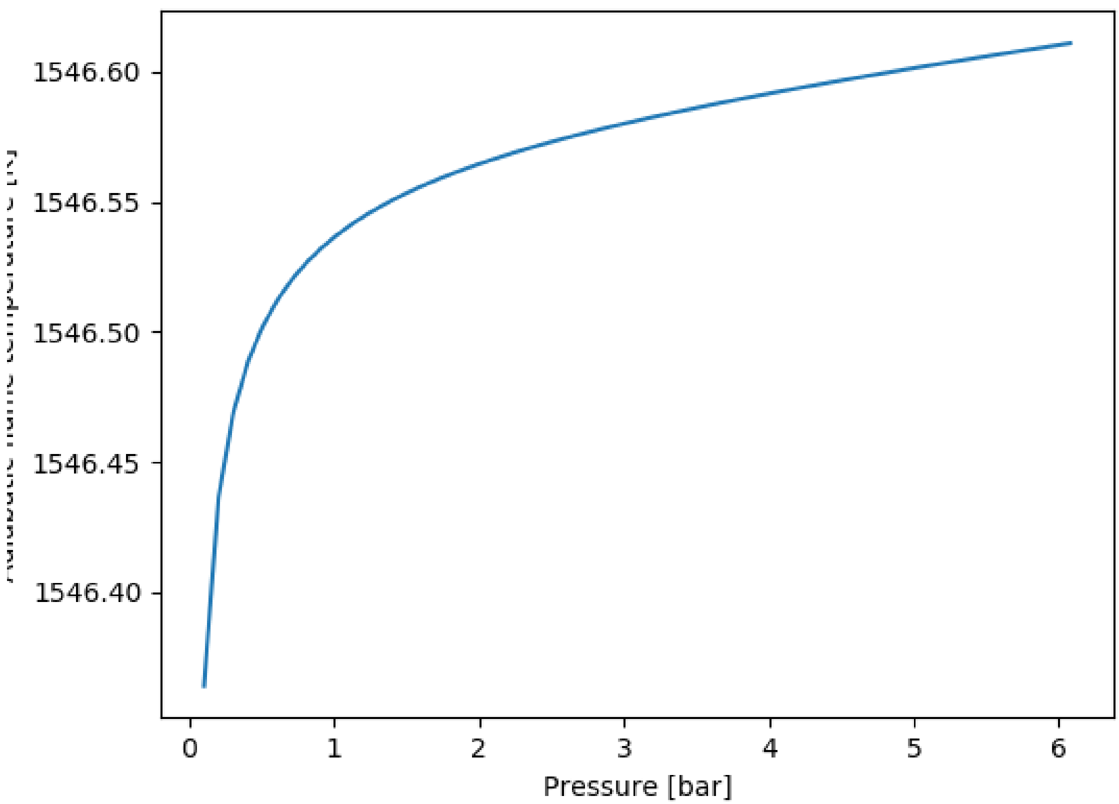

Figure 10: Methane

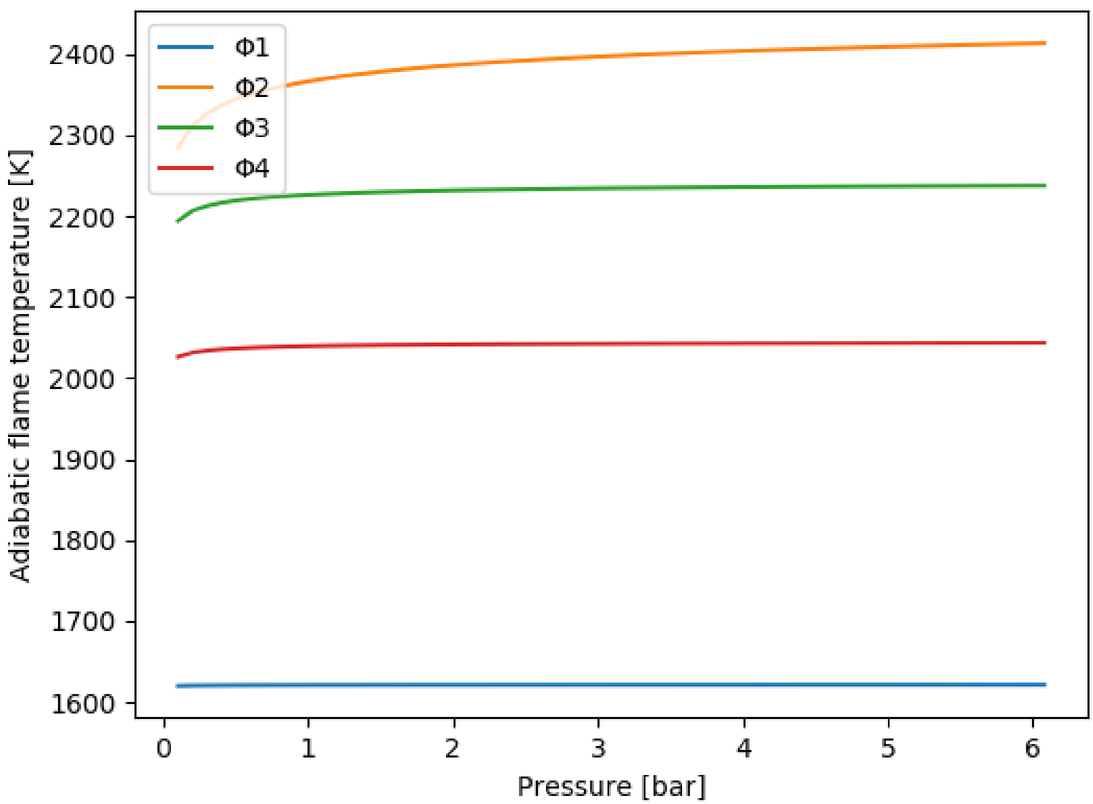

Figure 11: Hydrogen

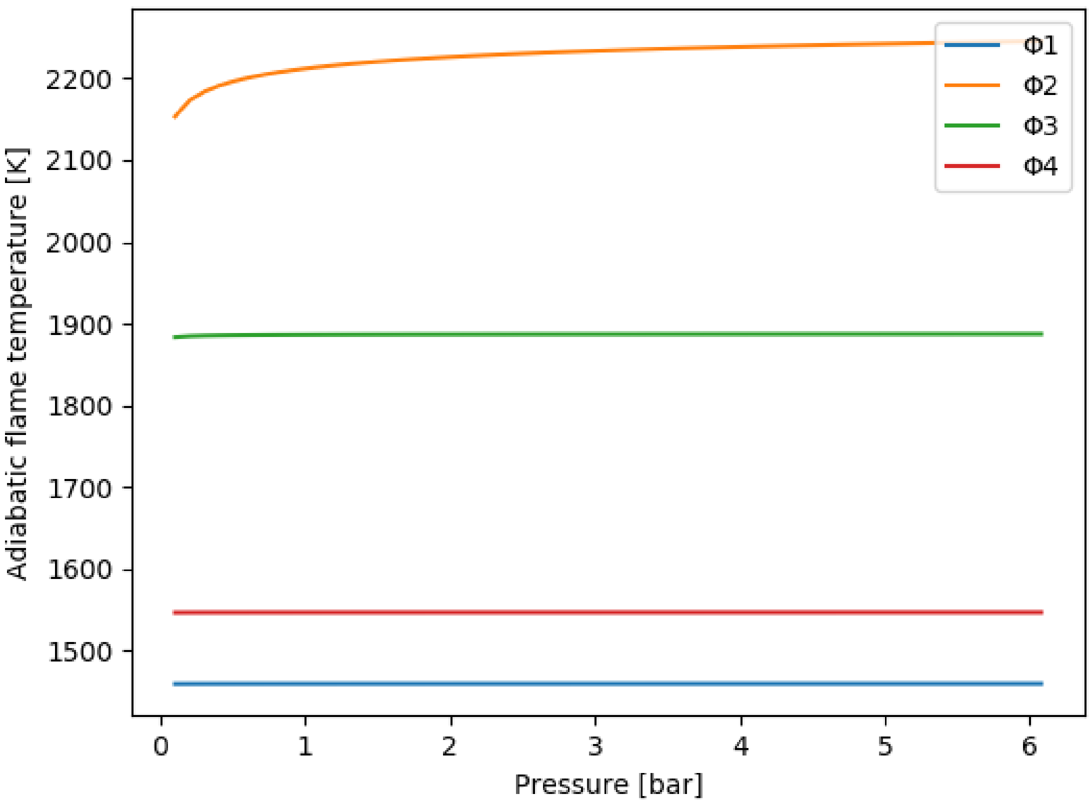

Figure 12: Methane

4.3 Variable P

Figures 13 to 22 present the counted relation between the adiabatic flame temperature and the initial value of pressure for four different equivalence ratios of methane-air mixture and hydrogen-air mixture. The initial temperature is $300[K]$.

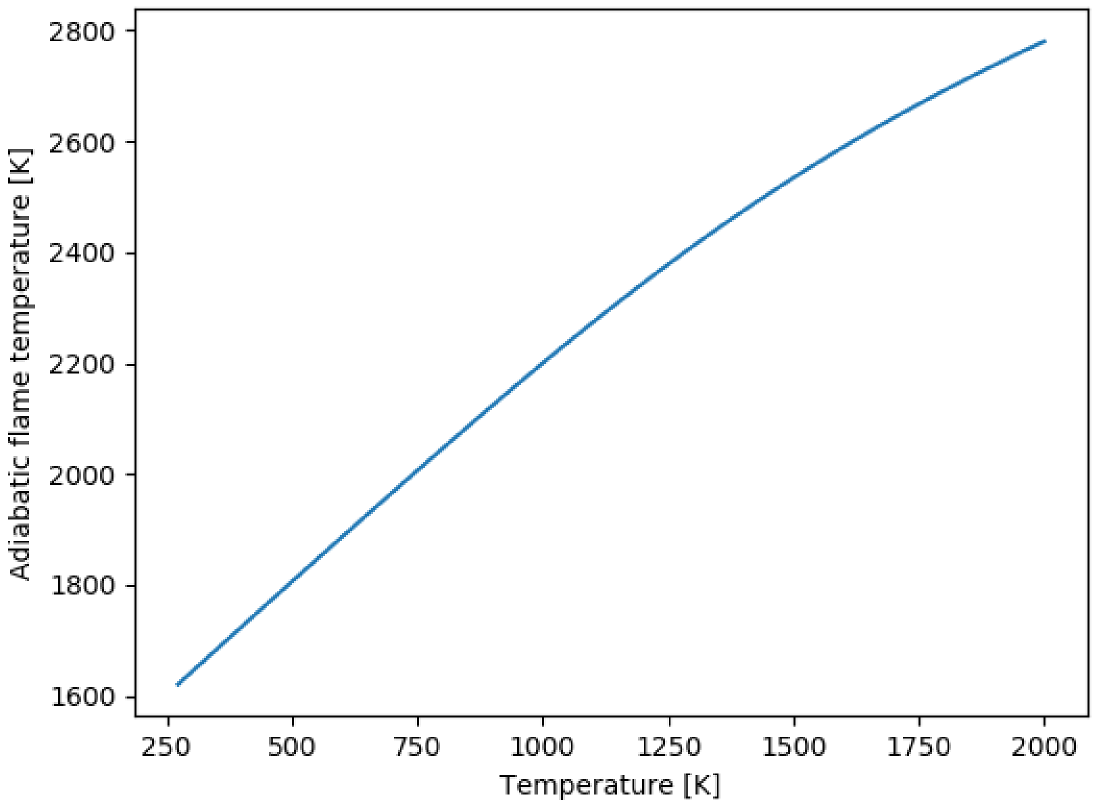

Figure 13: Hydrogen

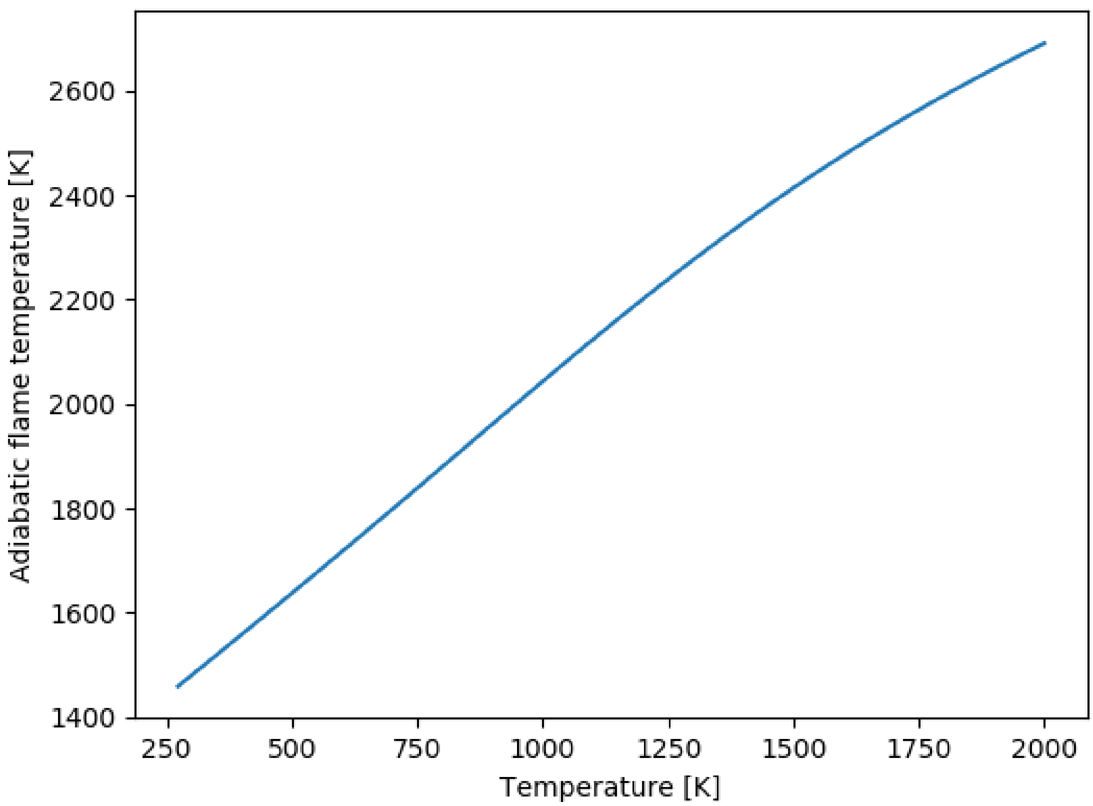

Figure 14: Methane

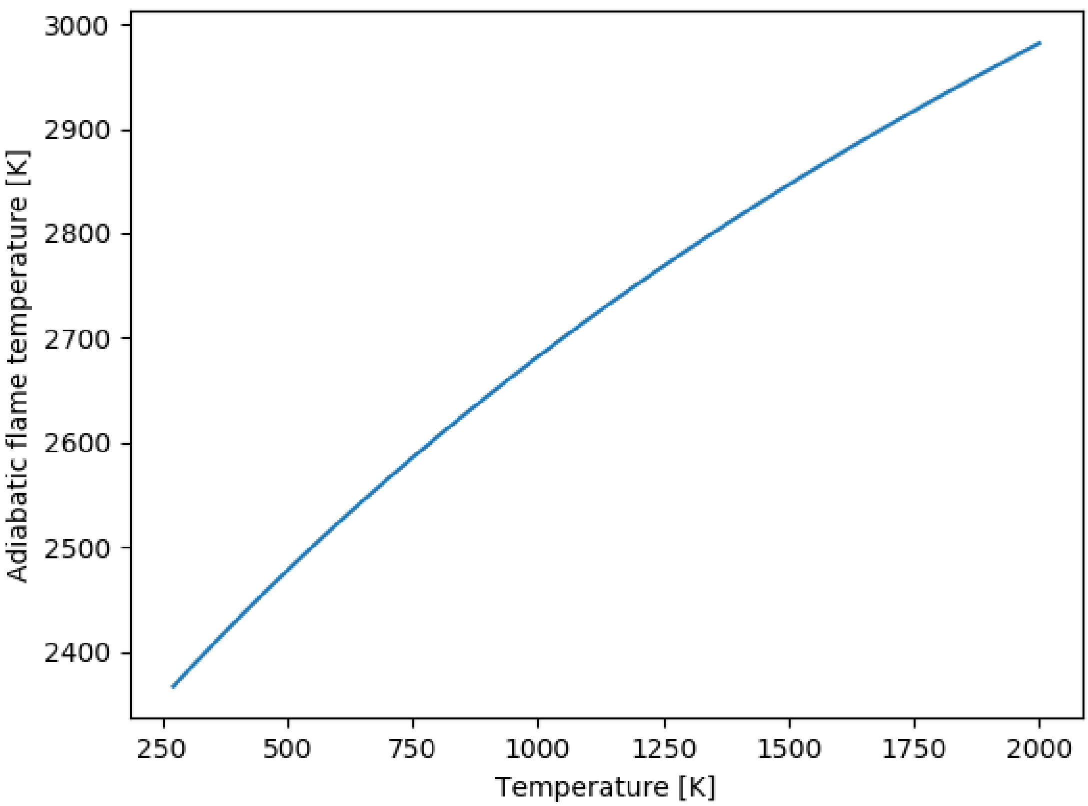

Figure 15: Hydrogen

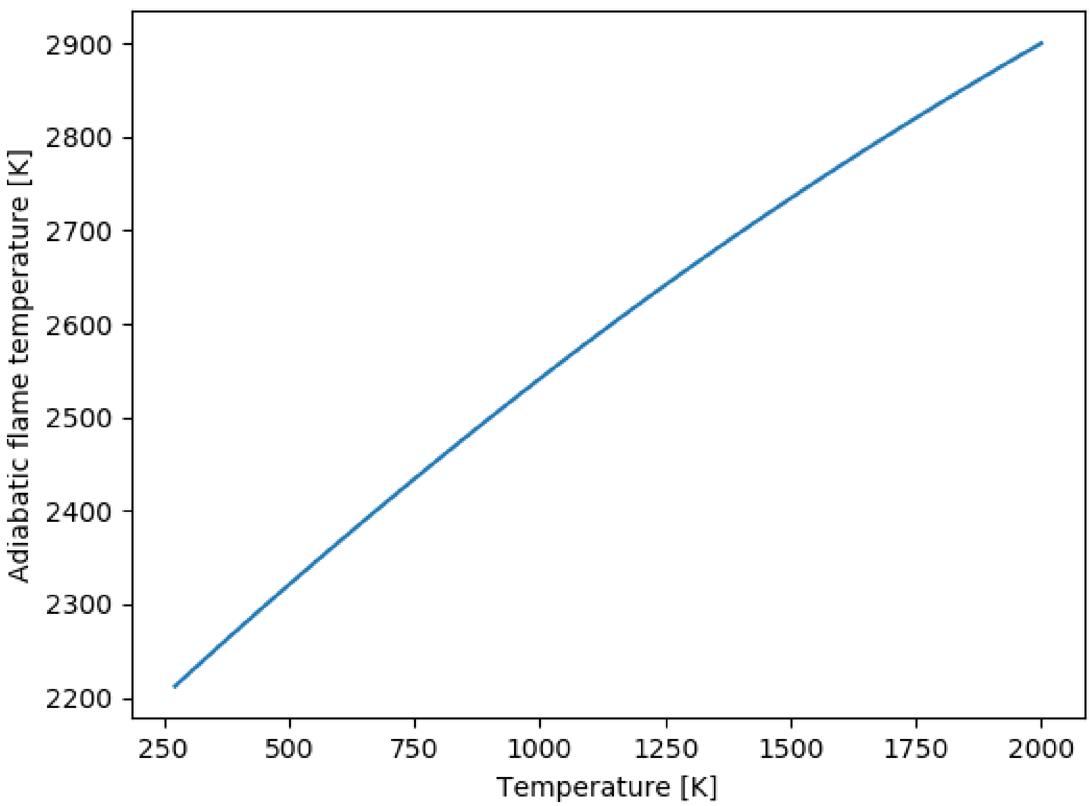

Figure 16: Methane

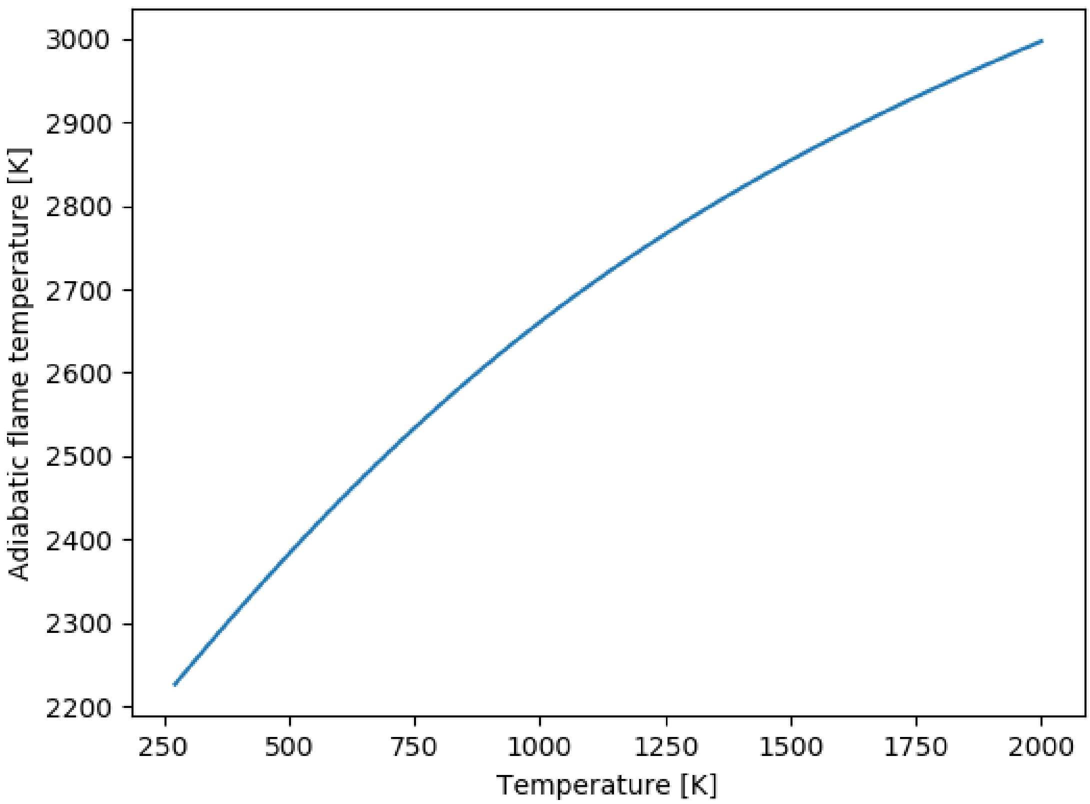

Figure 17: Hydrogen

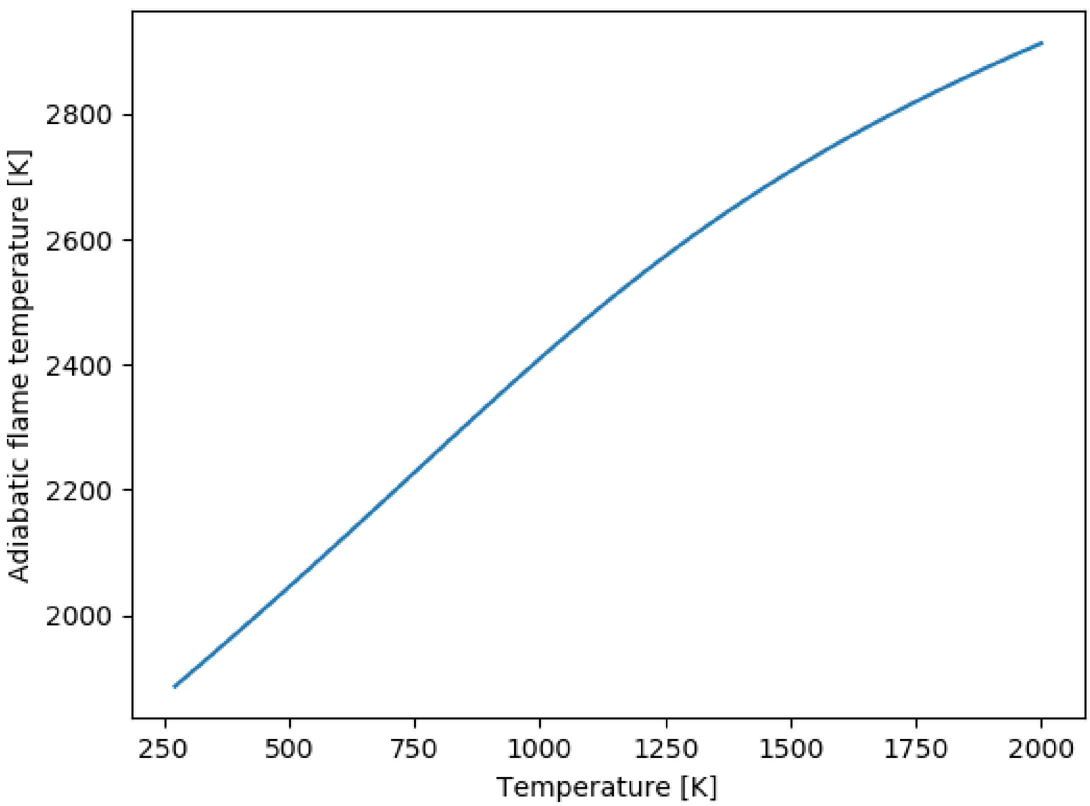

Figure 18: Methane

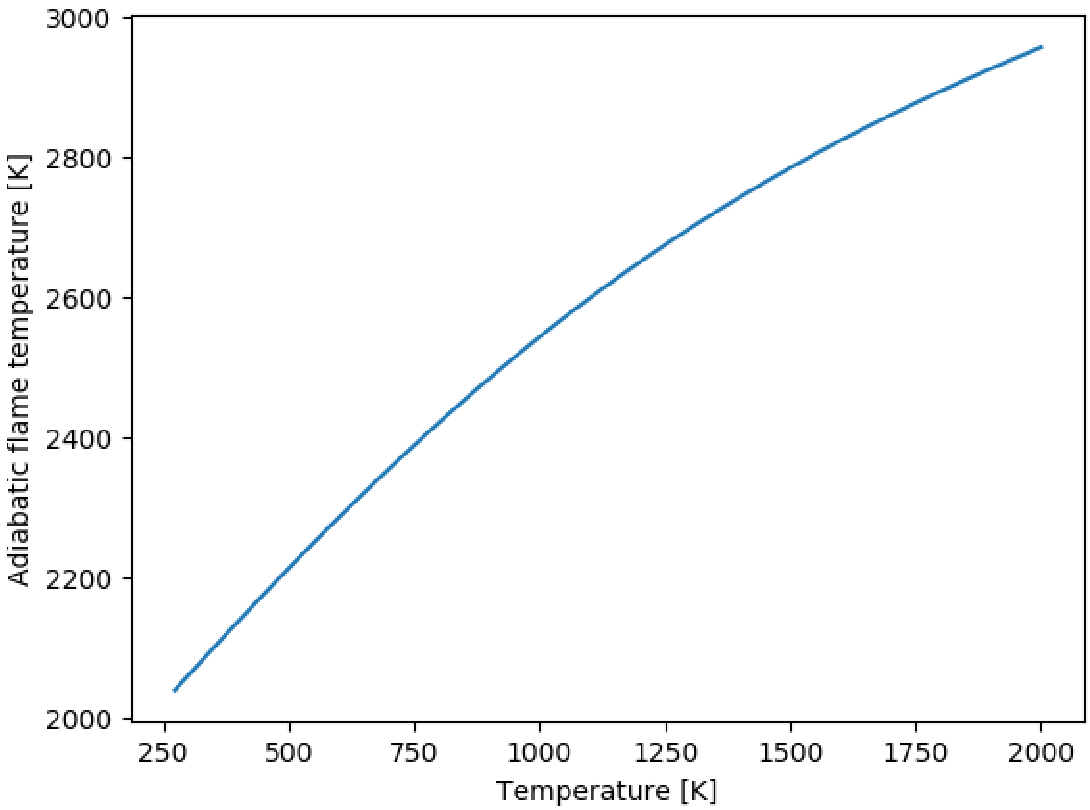

Figure 19: Hydrogen

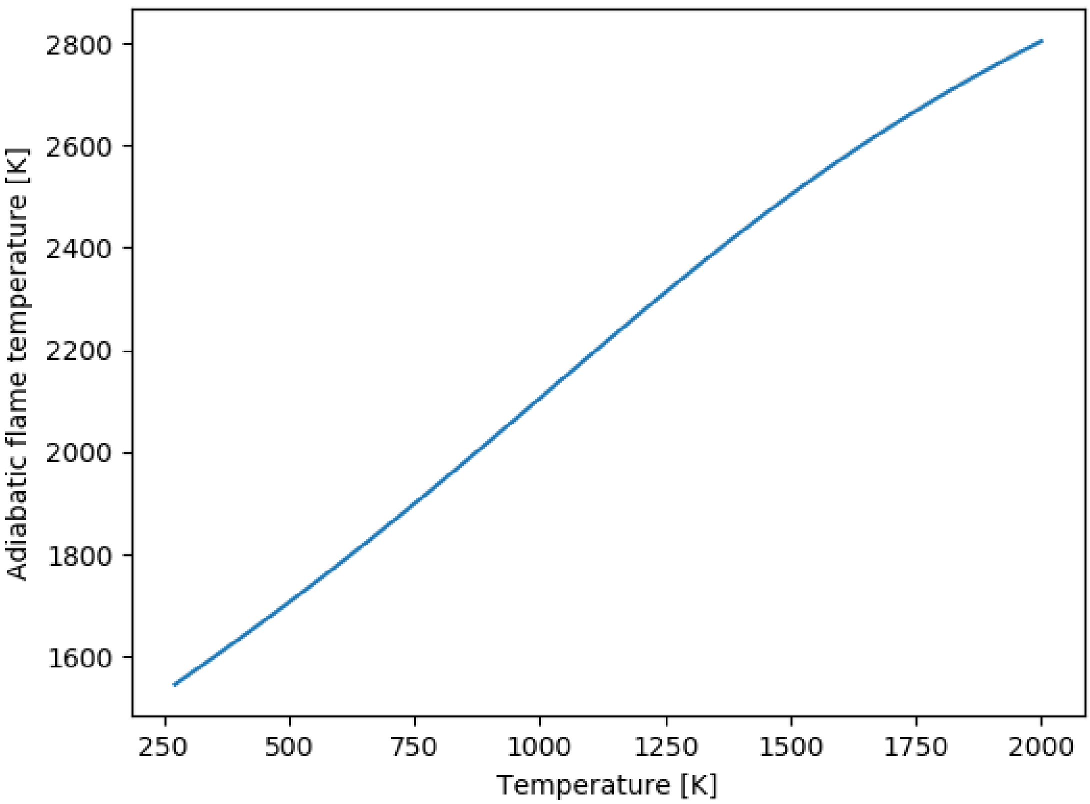

Figure 20: Methane

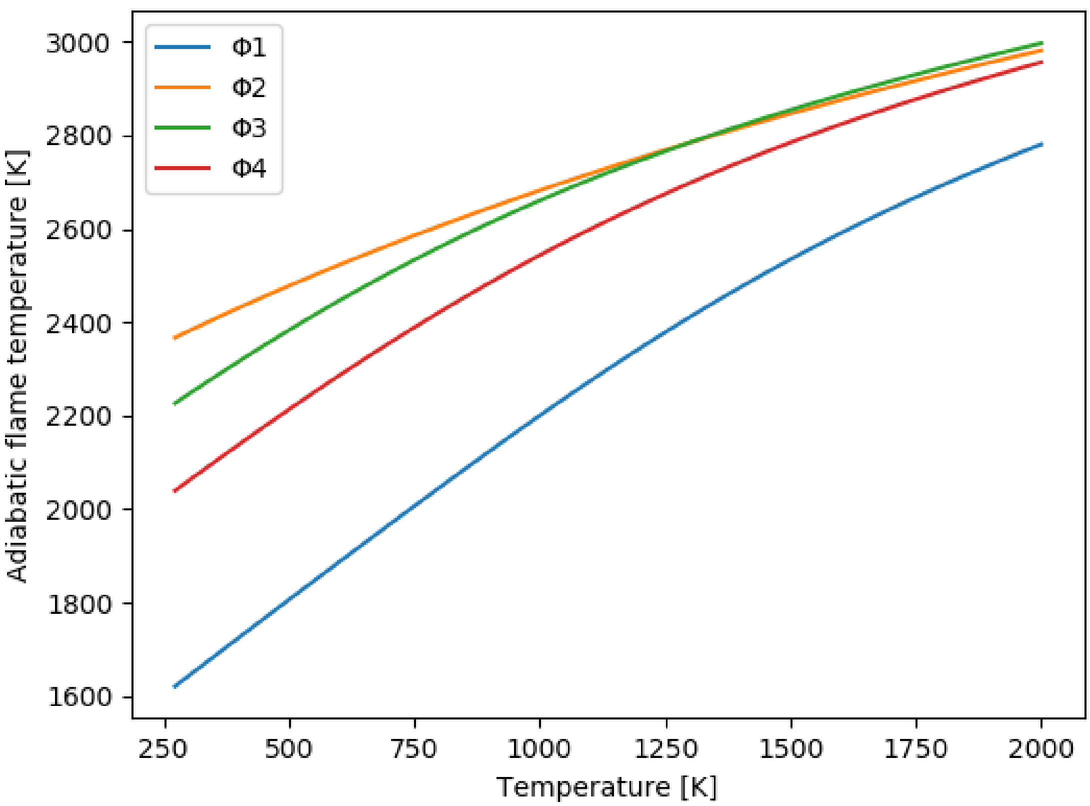

Figure 21: Hydrogen

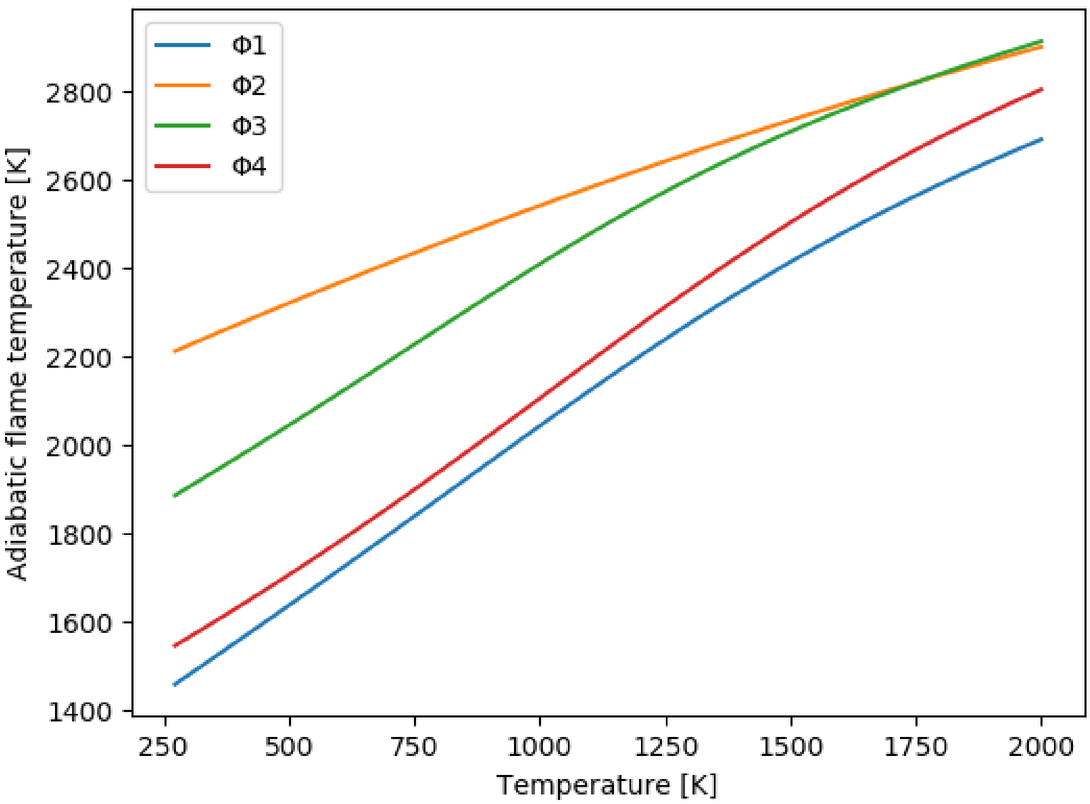

Figure 22: Methane

5 Conclusion

For both gases for constant initial pressure and temperature the highest temperature of adiabatic flame is reached when the composition of the mixture is slightly above the stoichiometric composition - the equivalence ratio is equal to one. For hydrogen decrease of temperature due to higher equivalence ratio is less radical than in case of methane. The temperature from hydrogen combustion is always able to achieve higher values then temperature from methane combustion for every starting conditions. The hydrogen can always achieve higher value of temperature for the same starting conditions to all temperature and pressure. In hydrogen combustion with $\Phi = 0.5$ is reducing temperature of flame drastically in comparison with $\Phi = 2$, when in case of methane has similar impact.

References

[1] Effects of equivalence ratio, pressure and preheat on adiabatic flame temperature. `https://github.com/majanus/MKWS`.

[2] Wojciech JERZAK. Adiabatic flame temperature and laminar burning velocity of ch4/h2/air mixtures (in polish). *Archiwum spalania*, Vol. 11:197–206, 08 2012.