Analysis of the adiabatic temperature and the temperature with constant volume in hydrogen air mixture combustion with different initial conditions

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Computational Methods in Combustion

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1 Introduction

Hydrogen is a chemical compound represented by the chemical formula H2. It is commonly used in many laboratories as very useful in the Laminar Burning Velocity studies and in the flame structure analysis whatsoever. Hydrogen is very explosive with the air as the oxidizer. Explosion of hydrogen-air mixture can be reached, when the hydrogen concentration is 4 to 75 percents.The goal of this study is to plot adiabatic temperature and temperature with constant volume of combustion connections depending on the initial temperature and pressure and concentration of hydrogen in air. In order to complete the calculations Cantera was used.

1.1 Stoichiometric equation

Stoichiometric equation representing hydrogen-air combustion is given as followed:

$$H_2 + 0.5(O_2 + 3.76N_2) = H_2O + 1.88N_2$$

1.2 Initial parameters

Initial temperature and pressure vary between:

$$T_0 = 273 - 2000\ [K]$$

$$p_0 = 1 - 5\ [bar]$$

Assumed initial concentrations:

$$\phi_0 = 0.5$$

$$\phi_1 = 1$$

$$\phi_2 = 2$$

$$\phi_3 = 3$$

$$\phi_4 = 4$$

2 Model

Using Cantera the basic reactor and gas models were prepared. Anacoda was used to obtain the necessary characteristics. All the simplifications and assumptions of the model are in line with those adopted in Cantera (e.g. the gas model is ideal, the combustion chamber is determined by the program conditions etc.).

3 Results

3.1 Temperature as function of initial pressure at constrained initial temperature

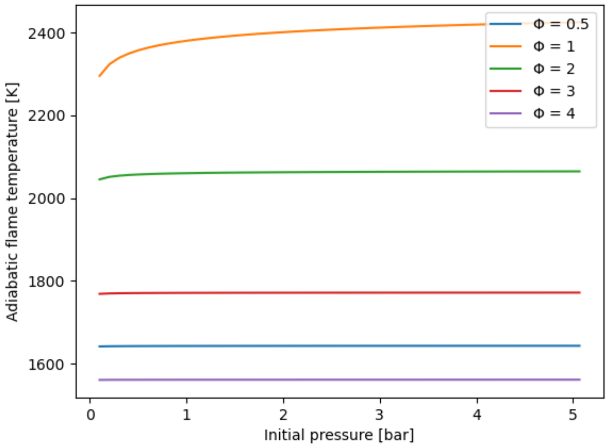

Figure 3.1.1: Adiabatic flame temperature for $T_0 = 273$ $[K]$

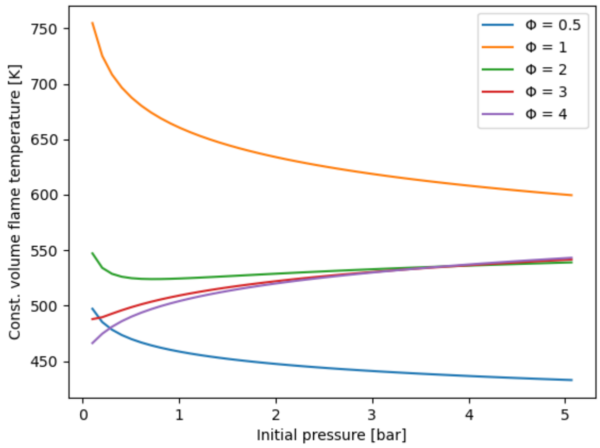

Figure 3.1.2: Flame temperature with constant volume $T_0 = 273$ $[K]$

Above figures show adiabatic flame temperature (Fig. 3.1.1) and flame temperature with constant volume (Fig. 3.1.2) as function of initial pressure with $T_0 = 273$ $[K]$. It's noticed that adiabatic flame temperature is almost independent of initial pressure, but it strongly depends of mixture's concentration.

In contrast, flame temperature with constant volume is strongly dependant of initial pressure. For mixtures with $\phi = 0.5$ and $\phi = 1$ concentration plays vial role in resulting temperature, but for $\phi = 2$, $\phi = 3$ and $\phi = 4$ temperature is almost the same.

3.2 Temperature as function of initial temperature at constrained initial pressure

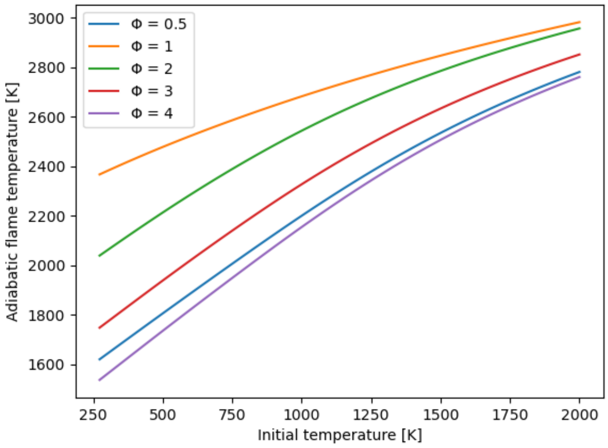

Figure 3.2.1: Adiabatic flame temperature for $\mathrm{p}_0 = 1$ $[bar]$

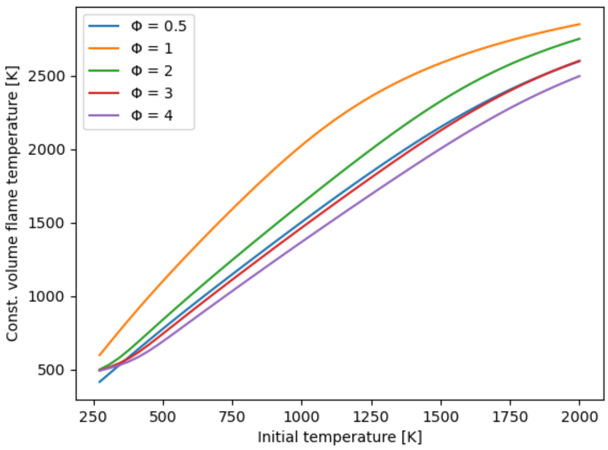

Figure 3.2.2: Flame temperature with constant volume $\mathrm{p}_0 = 1$ $[bar]$

Above figures show adiabatic flame temperature (Fig. 3.1.1) and flame temperature with constant volume (Fig. 3.1.2) as function of initial temperature with $p_0 = 273$ $[bar]$. It's noticed that adiabatic flame temperature is dependent of both initial temperature and mixture's concentration.

Having insight into flame temperature with constant volume it can be assumed that for all concentrations except $\phi = 1$ waveform of plot is very similar and is strongly dependent on initial temperature.

3.3 Adiabatic flame temperature as function of initial temperature and initial pressure for constrained concentration

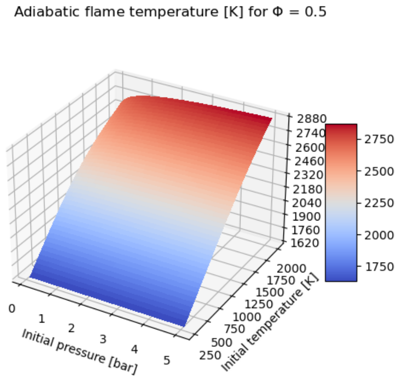

Figure 3.3.1: For $\phi = 0.5$

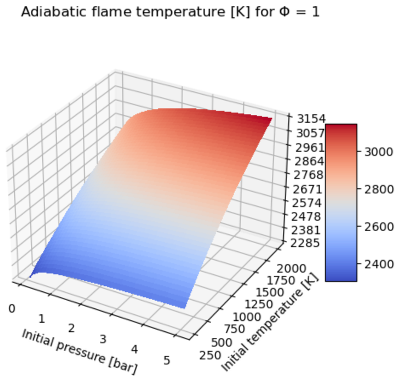

Figure 3.3.2: For $\phi = 1$

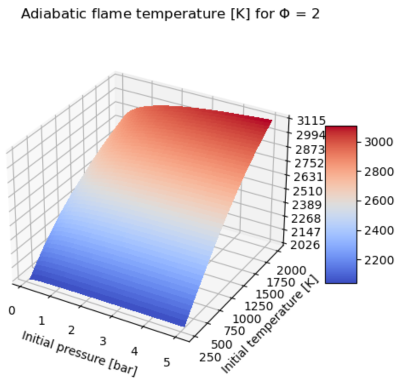

Figure 3.3.3: For $\phi = 2$

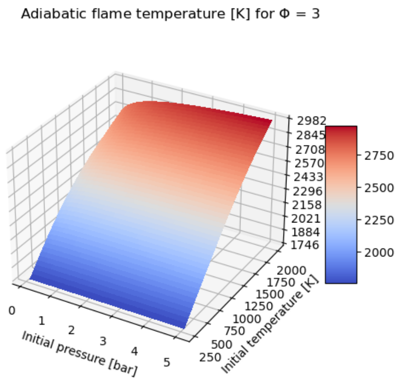

Figure 3.3.4: For $\phi = 3$

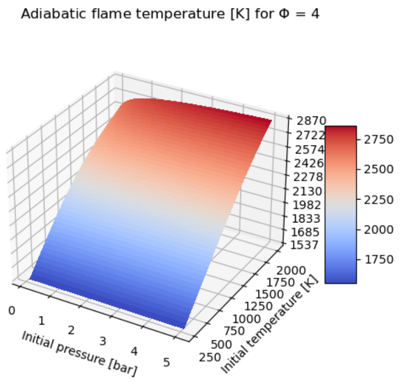

Figure 3.3.5: For $\phi = 4$

Above figures shows 3D plots of adiabatic flame temperature in function of initial pressure and initial temperature. It can be spotted that the highest maximum temperature is achieved form $\phi = 1$ (Fig. 3.3.2). For every concentration it's clear that initial temperature has greater impact on resulting temperature than initial pressure.

3.4 Flame temperature with constant volume as function of initial temperature and initial pressure for constrained concentration

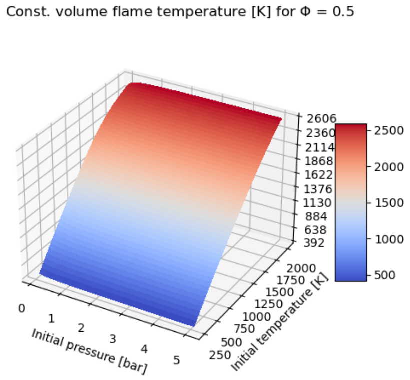

Figure 3.4.1: For $\phi = 0.5$

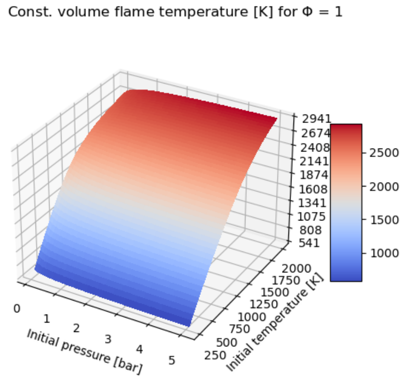

Figure 3.4.2: For $\phi = 1$

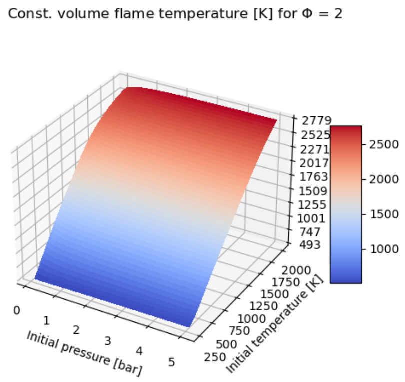

Figure 3.4.3: For $\phi = 2$

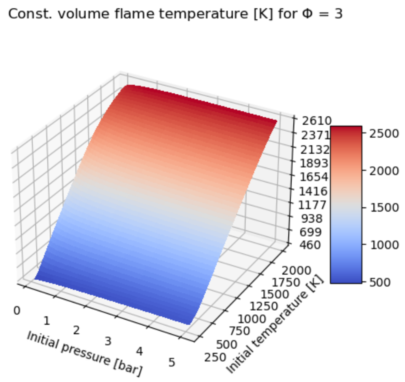

Figure 3.4.4: For $\phi = 3$

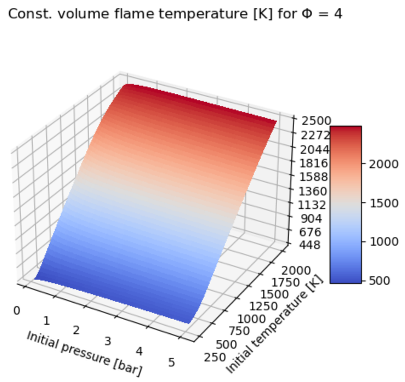

Figure 3.4.5: For $\phi = 4$

Above figures shows 3D plots of flame temperature with constant volume in function of initial pressure and initial temperature. It can be spotted that the highest maximum temperature is achieved form $\phi = 1$ (Fig. 3.4.2). For every concentration it's clear that initial temperature has greater impact on resulting temperature than initial pressure.

4 Summary

The purpose of this report was to examine the influence of the initial pressure, initial temperature and mixture concentration on adiabatic flame temperature and flame temperature with constant volume.

Considering all figures, It seems that both adiabatic flame temperature and temperature with constant volume have the greatest value for stoichometric mixture, $\phi = 1$.

Fig. 3.1.1 shows that adiabatic flame temperature for $T_0 = 273[K]$ is pressure independent (independent means, has less impact on combustion temperature), It can be noticed also on 3.3.1 - 3.3.5, for all condensations temperature is pressure independent, except $\phi = 1$.

Fig. 3.1.2 depicts that flame temperature with constant volume also is pressure independent.

Fig. 3.2.1 - 3.2.2 shows influence of initial temperature on both kind of combustion. Explicitly It has grater impact on combustion temperature than initial pressure.

To sum up, in both kinds of combustion i.e. adiabatic and with constant volume, temperature increases along with increase of initial conditions.

5 References

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   `https://github.com/AndrzejFurmanski/-MKWS2019---Cantera`
2. Marian Gieras, *Spalanie - wybrane zagadnienia w zadaniach*, 2011
3. `https://en.wikipedia.org/wiki/Air`
4. `https://en.wikipedia.org/wiki/Hydrogen`