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Computational Methods in Combustion

Adiabatic temperatures for hydrogen mixtures near LFL and
UFL

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1 Introduction

This project aims to show the differences between the adiabatic flame temperatures of hydrogen-oxygen and hydrogen-air mixtures. This study can be useful for further examination of the parameters of those mixtures and for checking the experimental data against the theoretical ones.

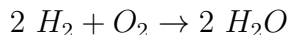
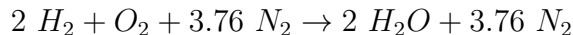
To compare those mixtures, two types of adiabatic flame temperatures were checked: adiabatic temperature at constant pressure (TAD_P) and adiabatic temperature at constant volume (TAD_VOL). In order to perform necessary calculations, the Python programming language and the Cantera library were used. Cantera is an open-source collection of object-oriented software tools for problems involving chemical kinetics, thermodynamics and transport processes.

Hydrogen mixtures have recently become the subject of many studies due to their flammable properties. Most notably, hydrogen combined with oxygen or air has a very wide flammability range. The flammability limits range from approximately 3.8% concentration of hydrogen in air and oxygen to about 75% in air and around 94% in oxygen. Moreover, the ignition activation energy of such mixtures is very low. Consequently, the burning velocity is high (approx. 2.9 m/s, while a methane flame spreads at approx. 0.4 m/s). These properties favor easy ignition but also pose the risk of uncontrolled explosions. Additionally, hydrogen molecules are small and have very low density. Therefore, they spread relatively quickly, which can lead to accidental explosions, e.g., due to leaks. As a result, storing hydrogen and handling hydrogen mixtures (their adiabatic temperatures) remains a significant challenge for engineers aiming to implement them in fields such as aviation or automotive technology.

The results of this project were used in further analysis performed during the pre-bachelor diploma.

2 Theoretical background

First, let's define the quantities used in this project and describe the relevant phenomena. The stoichiometric equations for the examined reactions are as follows:



The following terms are defined for the topic: explosion, explosion and flammability parameters, and the adiabatic temperature.

Explosion, explosion and flammability parameters

An explosion is a type of physical or chemical transformation of substances that causes a sudden change in the equilibrium state of the system. It is accompanied by the release of energy capable of performing mechanical work. A characteristic feature is the sudden increase in pressure in the medium surrounding

the explosion.

- **Lower Flammability Limit (LFL)** – the lowest concentration of flammable component in the mixture with the oxidizer below which the mixture ceases to be explosive, and above which flame propagation can occur.
- **Upper Flammability Limit (UFL)** – the highest concentration of flammable component in the mixture with the oxidizer above which the mixture ceases to be explosive, and below which flame propagation is possible.
- **Maximum Explosion Pressure** – the highest pressure generated during the explosion in a closed vessel with optimal fuel concentration and initial pressure of 0.1013 MPa.
- **Maximum Rate of Pressure Rise** – the highest rate of pressure increases during the explosion under the same conditions.
- **Optimal Explosive Concentration** – the fuel concentration in the oxidizer that results in the maximum pressure rise rate and minimum ignition limit.
- **Maximum Standard Rate of Pressure Rise (K)** – product of the maximum pressure rise rate, and the volume of the vessel used for the measurement.

To the group of basic gas flame parameters include e.g.: adiabatic temperature, autoignition temperature, flash point, autoignition delay time and laminar combustion velocity. For this study, we focus only on adiabatic temperature.

Ignition and extinction criterion

The ignition appears when the energy delivered to the gas (hydrogen here) is big enough to start the reaction (to reach the adiabatic temperature) and is being given to the volumetry of thickness at least the same of the laminar flame thickness. The speed of reaction needs to compensate for heat losses due to conduction of heat from the environment.

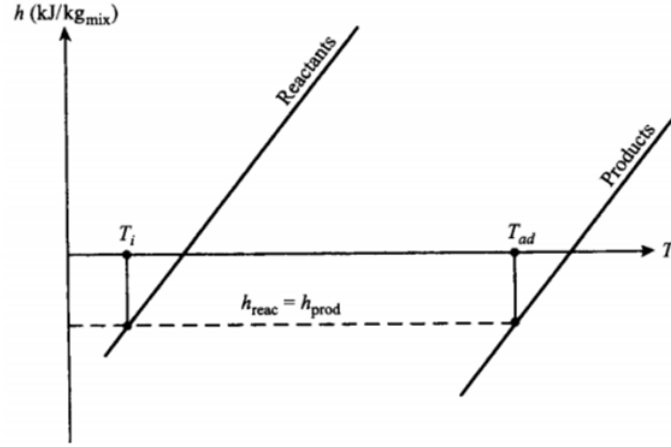
Adiabatic temperature

Adiabatic temperature is the temperature reached by a mixture after complete combustion with no heat exchange with the surroundings. It is an important parameter for e.g. combustion chamber constructors as it defines significant limitations for materials and the whole process as well. It limits the maximum temperature of exhaust gases.

The adiabatic temperature can be defined as adiabatic temperature at constant pressure and adiabatic temperature at constant volume. The first one is derived from the conservation of enthalpy rule:

$$H_{\text{reac}}(T_0, P) = H_{\text{prod}}(T_{\text{ad}}, P)$$

Figure 1:



And the second one from conservation of internal energy:

$$U_{\text{reac}}(T_0, P) = U_{\text{prod}}(T_{\text{ad}}, P)$$

It is worth mentioning that for the same initial parameters:

$$T_{\text{ADVOL}} > T_{\text{ADP}}$$

Knowing T_{ADVOL} , we can get the maximum explosion pressure. The T_{ADP} is fine for examination of exhaust gases, as we assume that there is no constant volume, only the pressure. To examine explosions in closed volumes and their parameters the T_{ADVOL} describe it properly.

3 Method description

The purpose of the simulation was to examine the adiabatic flame temperatures for both hydrogen-oxygen and hydrogen-air mixtures near to their LFL and UFL and check how does it changes with two initial parameters:

- Initial temperature T_0 – from 25°C to 100°C, changing each 5°C
- Concentration of hydrogen in the mixture, changing for each 0.25%:
 - 3–6% for both mixtures,
 - 75–85% for air,
 - 85–95% for oxygen.

The adiabatic flame temperature is defined by conservation of enthalpy rule, but Cantera finds it in numerical way solving:

$$\int_{T_0}^{T_{AD}} \sum_j n_j \bullet c_{pj}(T) \bullet dT = \Delta h_{mixture}$$

The Cantera library has the heat capacity c_p , enthalpy of the products and number of moles of products and reagents n . Thanks to `gas.equilibrate("HP")` Cantera finds temperature for which:

$$H_{mixture}(T) = H_{initial}$$

At constant pressure (“P”).

When it comes to constant volume, Cantera must find temperature for which:

$$U_{reac}(T_0, P) = U_{prod}(T_{AD}, P)$$

This is done also in numerical way with iterations. To initiate this type of combustion the `gas.equilibrate("UV")` was used, for constant volume (“V”).

To define the gas, the file `h2o2.yaml` was used as it stores all kinetic and thermodynamic data for reaction for hydrogen mixtures. Thanks to that file Cantera allows us to speed up the calculation.

The necessary loops were used to calculate temperatures for each initial temperature and concentration. For further study this can be changed.

The results were stored in array and in an excel file for further use. For each pair of T_0 - H_2 , T_{ADP} and T_{ADVOL} were calculated and stored in the array. To create the results as isotherms, Numpy meshgrid function was used.

4 Results and analysis

As a result, a few charts were created. The point of visualization was to create isotherms connecting pairs of T_0 - H_2 , for which T_{ADP} and T_{ADVOL} was the same, and compare the mixtures.

Figure 2:

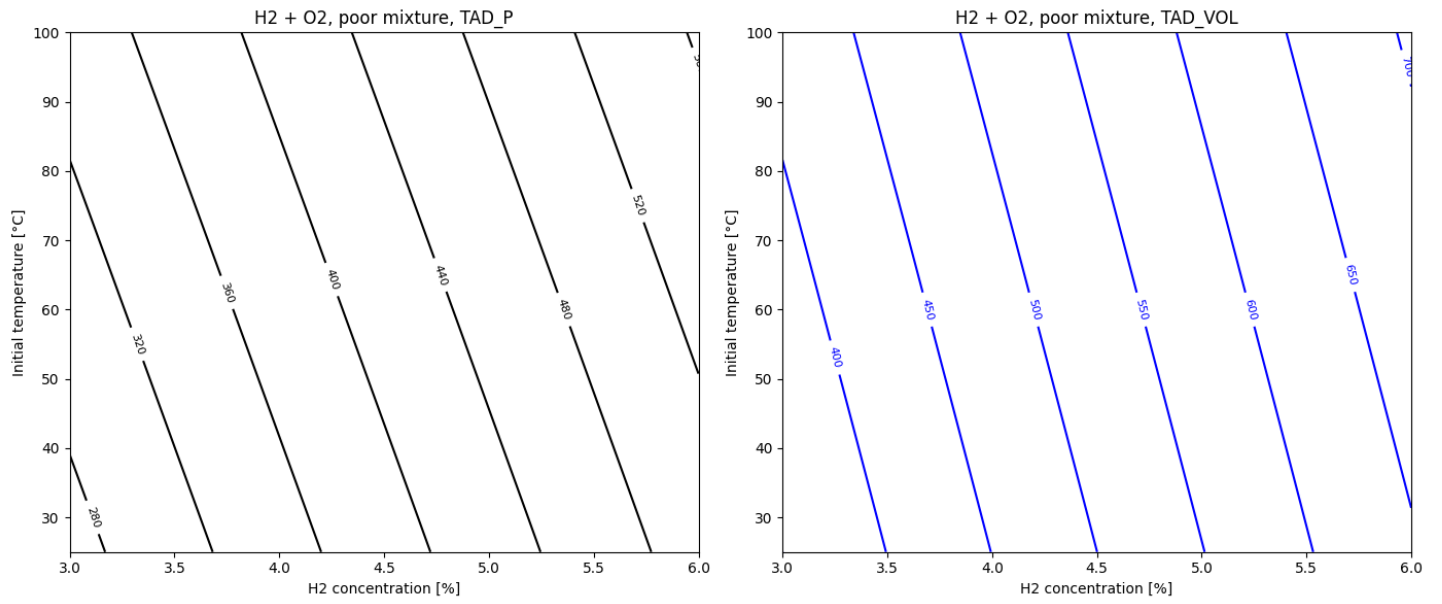


Figure 3:

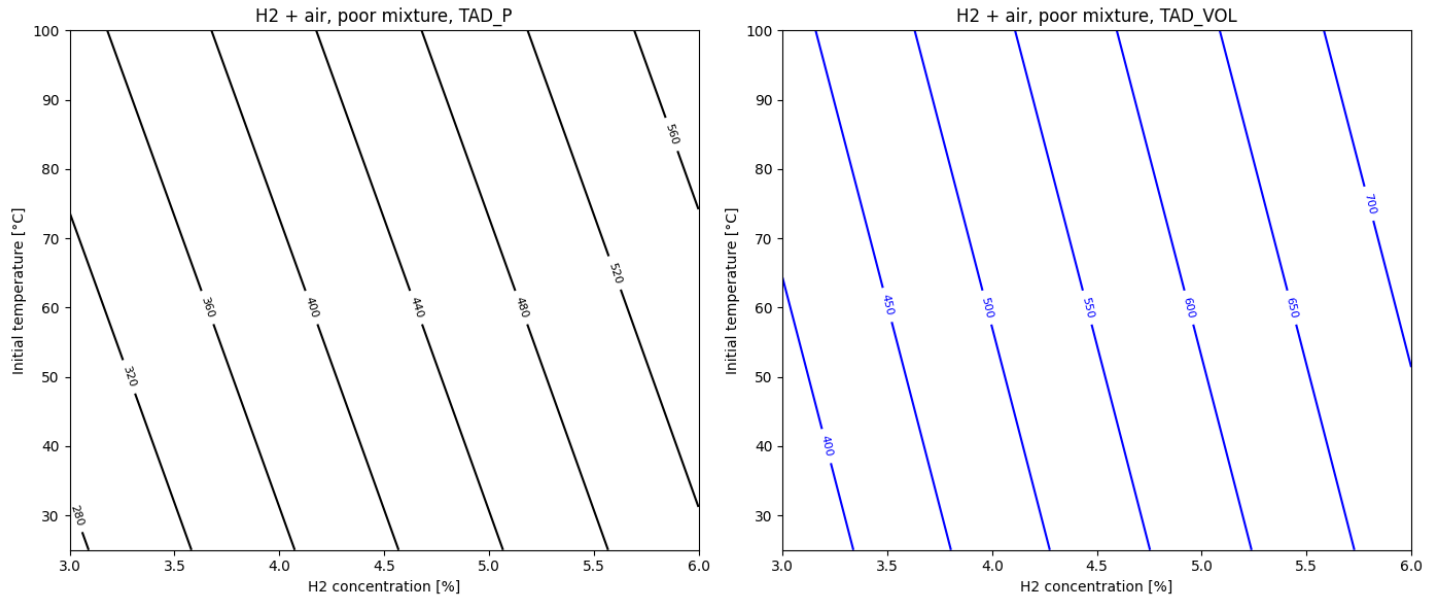


Figure 4:

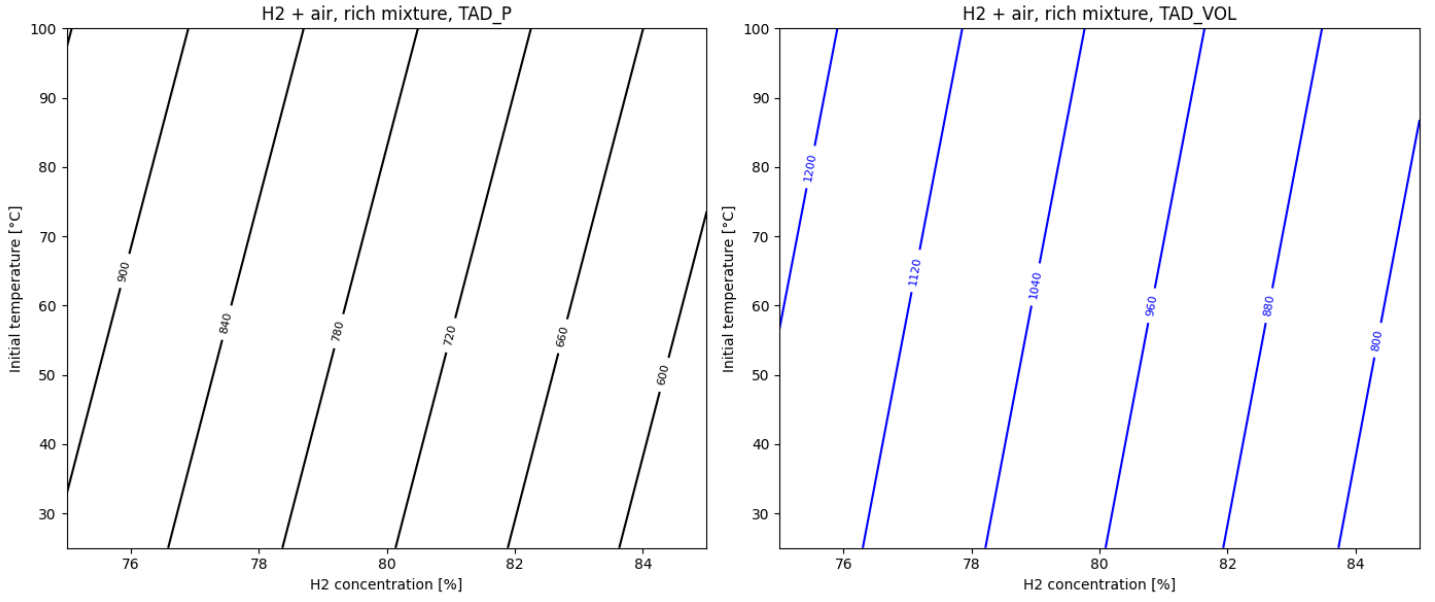
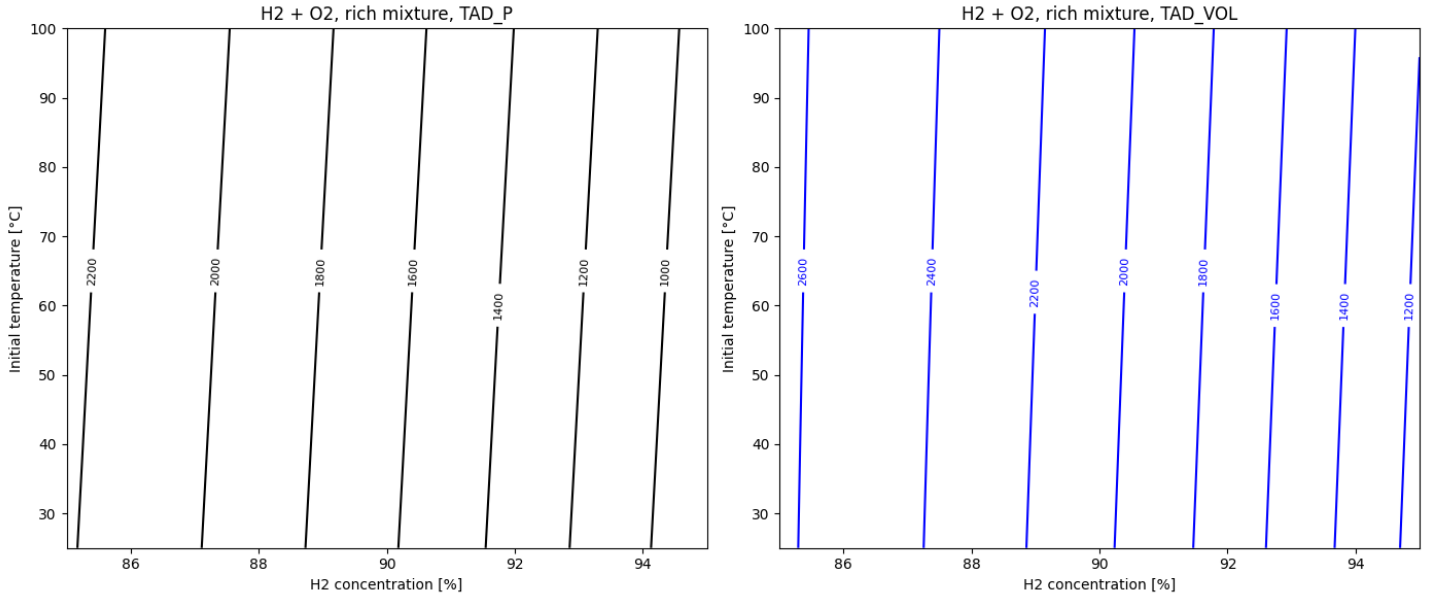


Figure 5:



5 Conclusion

What can be concluded from the figures above:

- The adiabatic temperature at constant volume is indeed bigger than adiabatic temperature at constant pressure.
- For concentration near LFL, the adiabatic temperature growth with concentration and initial temperature. Giving higher initial temperature we can get the same adiabatic temperature for lower concentrations and so on.

- The exact opposite can be noticed for concentrations near UFL – the adiabatic temperature gets lower with the concentration.
- The values of adiabatic temperature are higher for hydrogen-air mixture.
- The slope of the adiabatic temperature in the H₂-O₂ mixture is definitely lower for UFL than for air mixture.
- The direction and the slope of the isotherms indicate the growth of adiabatic temperatures which suggest parameters for stoichiometric reaction.

6 Bibliography

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