WARSAW UNIVERSITY OF TECHNOLOGY

FACULTY OF POWER AND AERONAUTICAL ENGINEERING

COMPUTATIONAL METHOD IN COMBUSTION

Combustion of Hydrogen-Oxygen mixture in rocket engine at various initial conditions

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1 Introduction

The purpose of this work is to determine parameters of combustion of Hydrogen-Oxygen mixture in a rocket engine. Calculations shall be performed at various initial conditions for the pressure and the temperature. The products of combustion will also be presented. Additionally, exhaust gas velocity shall be calculated and presented in relation to initial conditions. To model natural gas combustion, GRI-Mech 3.0 model shall be used, which is included in the Cantera package. The program will be written in Python.

2 Theoretical model

The rocket engine, considered in this work, is a liquid rocket engine. This means that both the fuel (hydrogen) and the oxidizer (oxygen) are stored separately, in liquid forms, in pressurized vessels. During firing, both are pumped into the combustion chamber, where they are ignited and burned. Hot exhaust gases then escape through the nozzle, thus propelling the rocket in the opposite direction in accordance to Newton's Third Law of Motion. A simplified schematic of a rocket engine is presented on Figure 1 below.

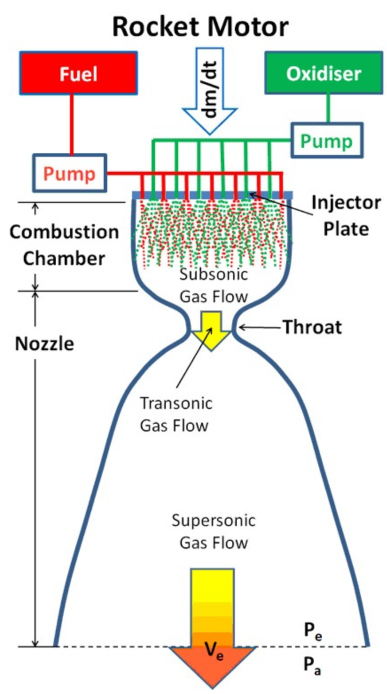


Figure 1: Liquid rocket engine schematic

In order to calculate properties of the combustion products, as well as their velocity, several assumptions have to made:

- Flow through the nozzle is isentropic,
- Fuel and oxidizer are pumped into the combustion chamber in gas form,
- The chamber is zero-dimensional
- Mass flow rate of fuel and oxidizer is constant.

With these assumptions, Cantera package can be used to determine properties of the exhaust gases. It is necessary to first determine the reaction formula. For hydrogen-oxygen combustion it is very simple:

$$2\,H_2 + O_2 \longrightarrow 2\,H_2O$$

Stechiometric mixture is assumed for the reaction.

2.1 Cases for initial conditions

Calculations were performed for different initial conditions listed below:

1. Case I
   (a) Temperature 300K
   (b) Pressure 5atm
2. Case II
   (a) Temperature 300K
   (b) Pressure 10atm
3. Case III
   (a) Temperature 300K
   (b) Pressure 20atm
4. Case IV
   (a) Temperature 300K
   (b) Pressure 50atm
5. Case V
   (a) Temperature 350K
   (b) Pressure 5atm
6. Case VI
   (a) Temperature 400K
   (b) Pressure 5atm
7. Case VII
   (a) Temperature 450K
   (b) Pressure 5atm
8. Case VIII
   (a) Temperature 500K
   (b) Pressure 5atm

3 Code overview

The program first initializes all of the reactants and what state they are in, namely their initial temperature, pressure and chemical composition. Next, combustion chamber and ignition mechanism are set up. The combustion chamber's virtual volume was set to $0,002m^3$. The reaction is started by injection of a small does of free hydrogen radicals. Next the program calculates the k coefficient, which is later used to determine the pressure difference between reservoirs. Mass flow depends only on the area of the throat section of the nozzle. The area of fuel injector, oxidizer injector and nozzle's throat are predetermined as follows:

$$A_{fuel} = 4e^{-4}m^2$$
$$A_{oxidizer} = 4e^{-4}m^2$$
$$A_{throat} = 5e^{-3}m^2$$

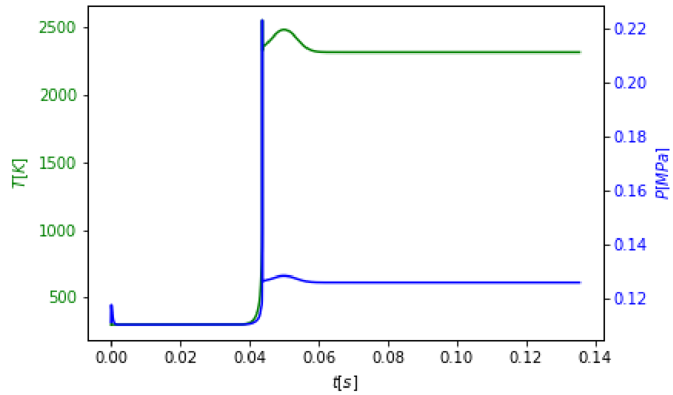
With these values set up in the code, the program then is capable of calculating the escape velocity of the reaction products, using the following equation:

$$V_2 = \sqrt{2T_c \frac{kR}{k-1}\left(1 - \left(\frac{p_2}{p_c}\right)^{\frac{k-1}{k}}\right)}$$

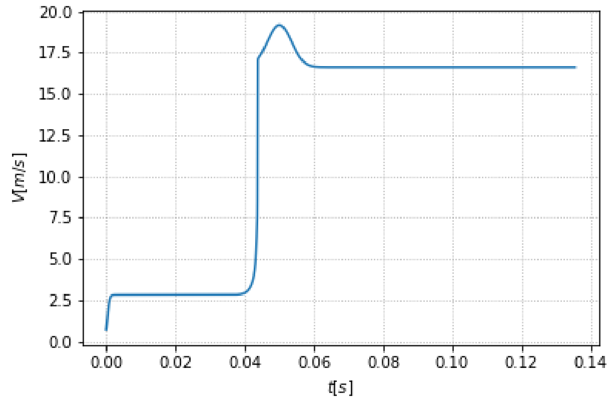
The state of the gases, namely the temperature, pressure and mass of each of the substrates and products, are calculated by Cantera functions. All parameters are then presented on charts, which are shown in the next section of this work.

4 Results

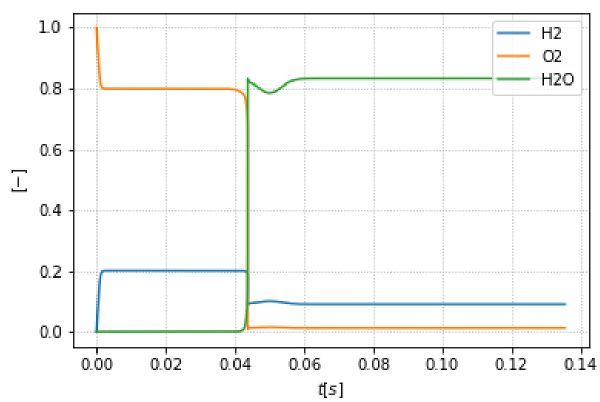
4.1 Case I



(a) Temperature and pressure graph



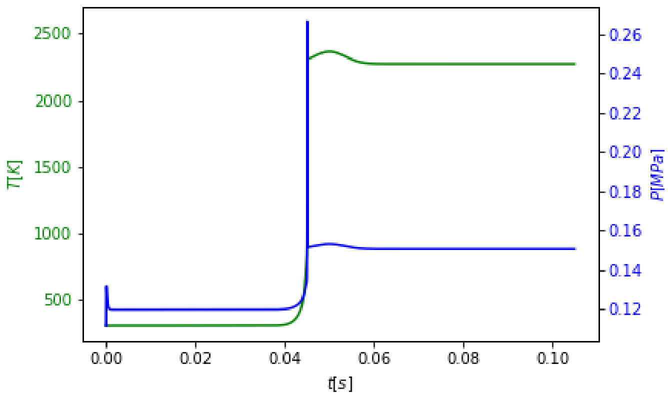
(b) Exit velocity of gases



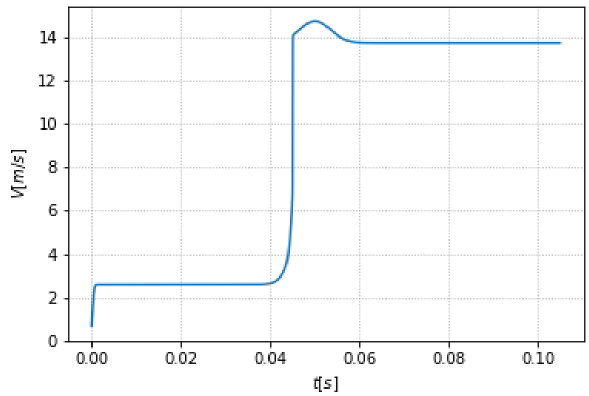
(c) Concentration of gases during reaction

Figure 2: Results for Case I

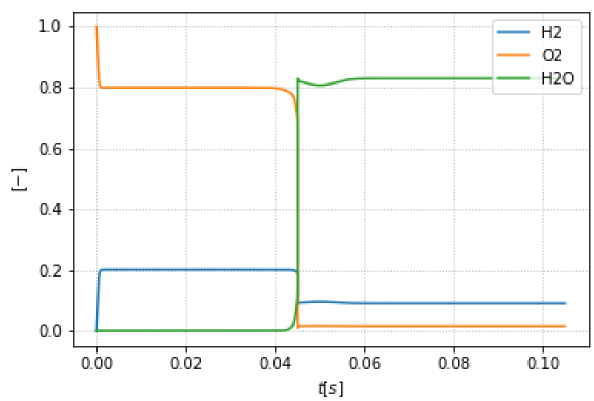
4.2 Case II



(a) Temperature and pressure graph



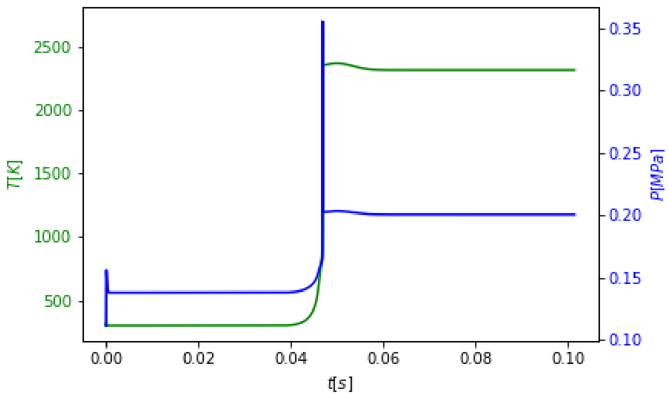
(b) Exit velocity of gases



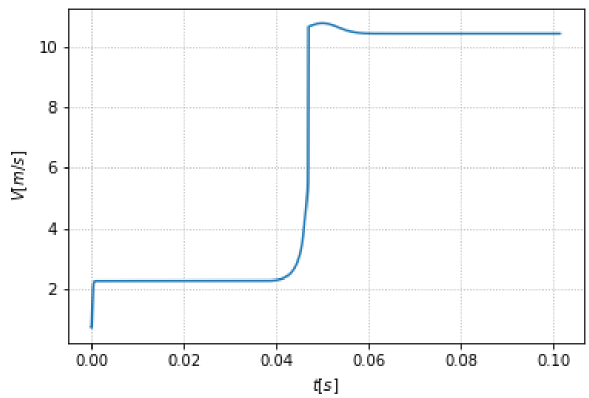
(c) Concentration of gases during reaction

Figure 3: Results for Case II

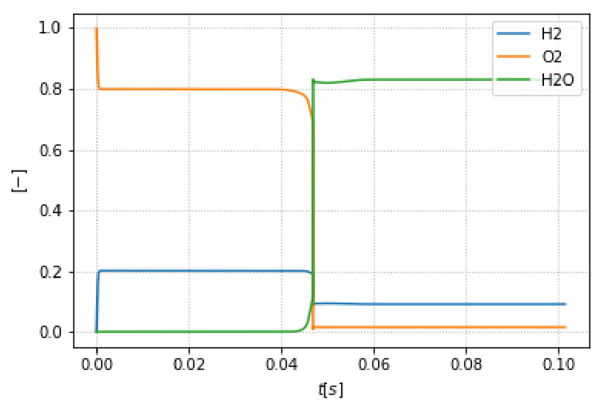
4.3 Case III



(a) Temperature and pressure graph



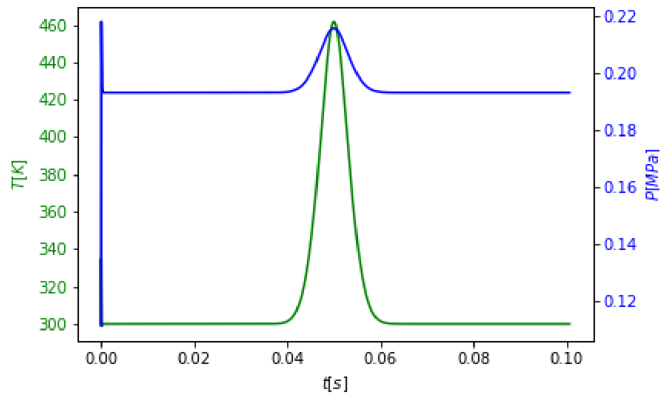
(b) Exit velocity of gases



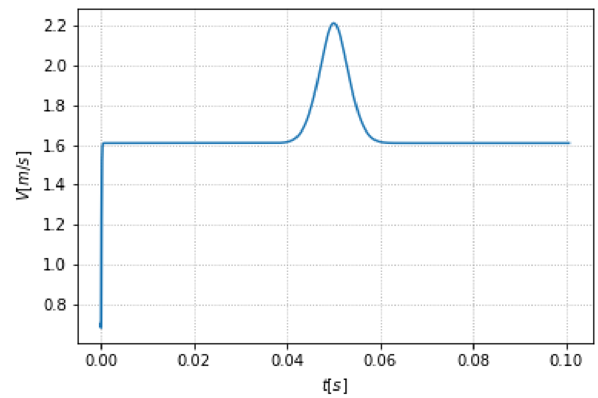
(c) Concentration of gases during reaction

Figure 4: Results for Case III

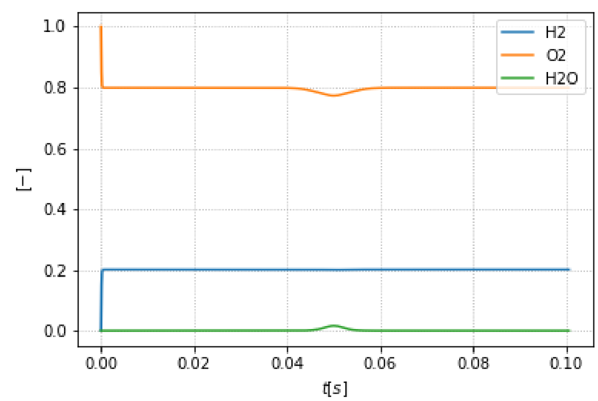
4.4 Case IV



(a) Temperature and pressure graph



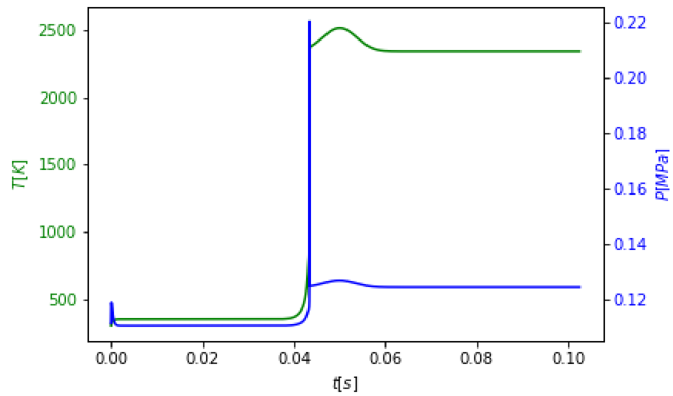
(b) Exit velocity of gases



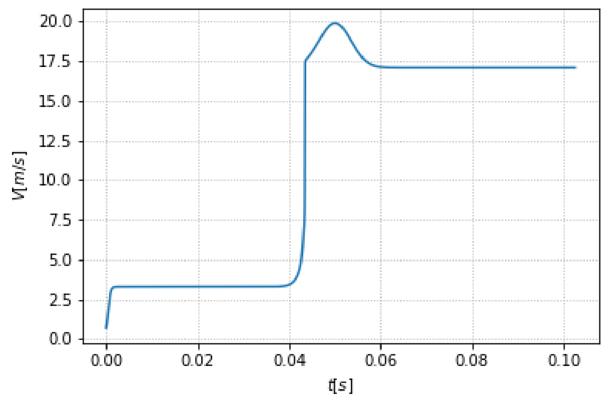
(c) Concentration of gases during reaction

Figure 5: Results for Case IV

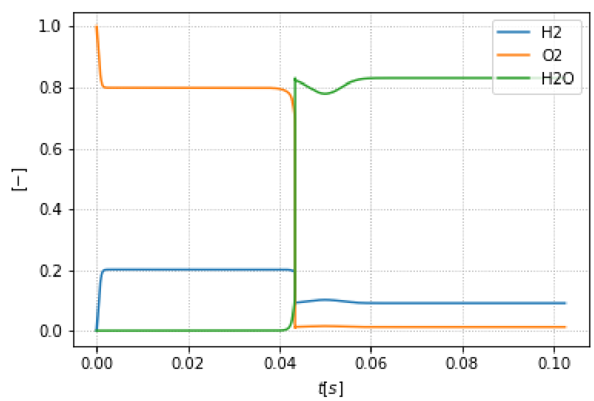
4.5 Case V



(a) Temperature and pressure graph



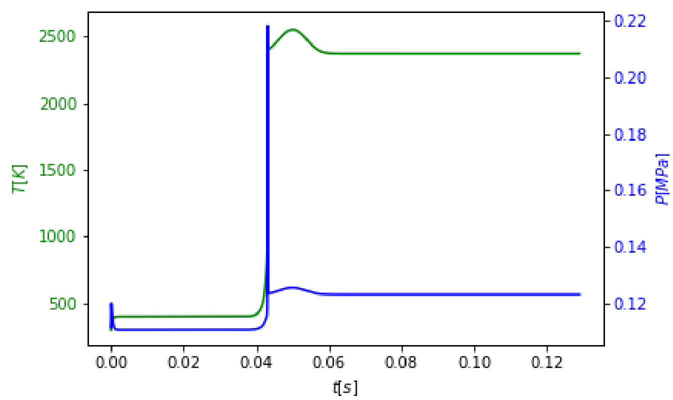
(b) Exit velocity of gases



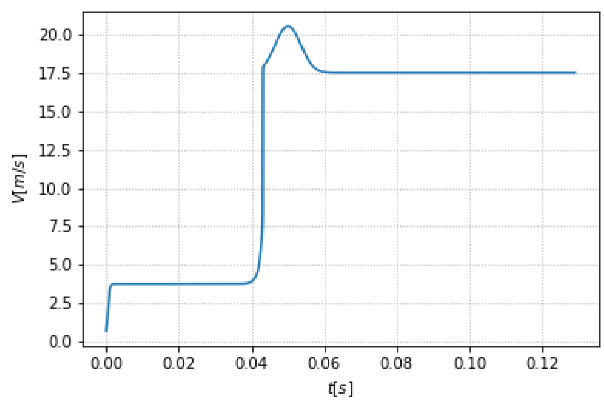
(c) Concentration of gases during reaction

Figure 6: Results for Case V

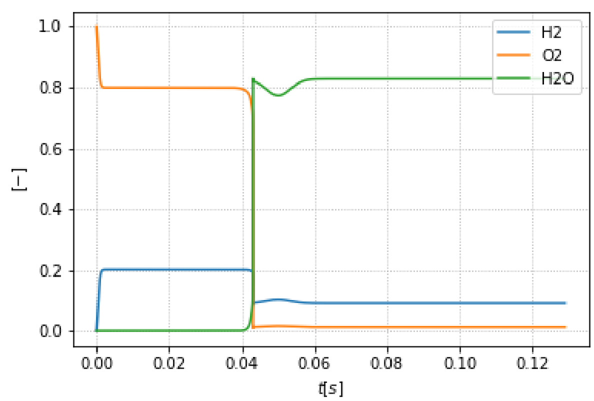
4.6 Case VI



(a) Temperature and pressure graph



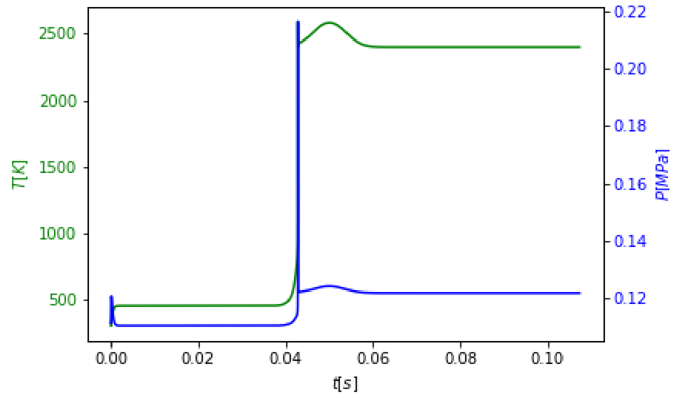
(b) Exit velocity of gases



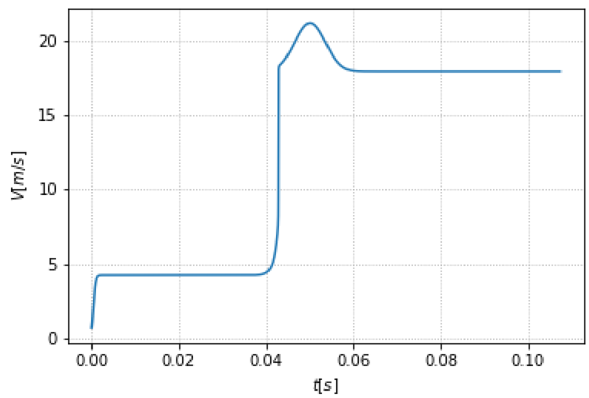
(c) Concentration of gases during reaction

Figure 7: Results for Case VI

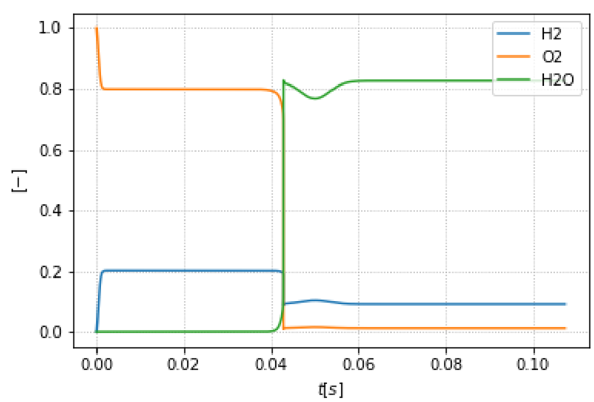
4.7 Case VII



(a) Temperature and pressure graph



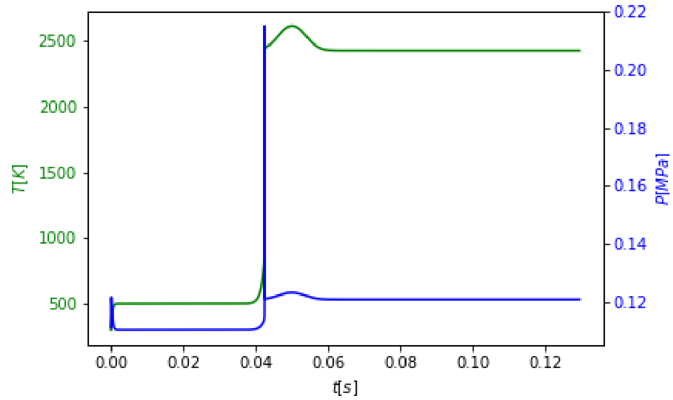
(b) Exit velocity of gases



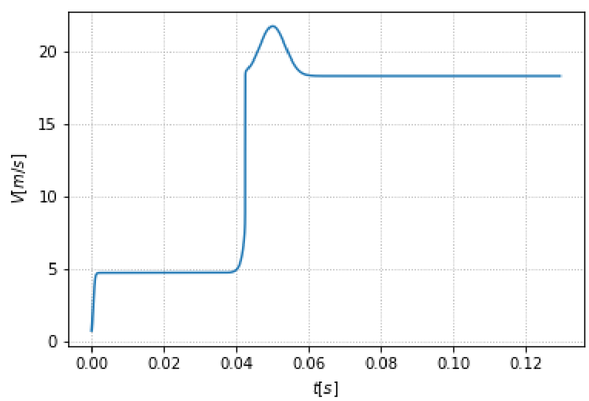
(c) Concentration of gases during reaction

Figure 8: Results for Case VII

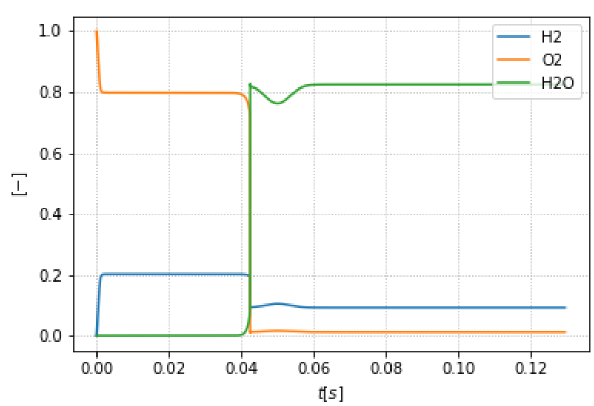
4.8 Case VIII



(a) Temperature and pressure graph



(b) Exit velocity of gases



(c) Concentration of gases during reaction

Figure 9: Results for Case VIII

5 Summary

As we can see from the graphs, there is a noticable increase in temperature and velocity of the gases that exit the nozzle after ignition. We also observe a spike in pressure of the gases, which reaches it's maximum at the moment of ignition, and then stabilizes at a lower value, which is higher than the initial pressure. As we could have expected, after ignition the concentration of oxygen and hydrogen decreases, while the concentration of H_2O increases. It is worth noting though, that the concentration of H_2 does not reach zero, like we might have expected, since the reaction is stechiometric. This is caused by the way the mixture is ignited. We added free hydrogen radicals, which in turn slightly increased the initial hydrogen concentration. These did not take part in the reaction due to insufficent oxygen in the mixture.

It can be observed, that with increased initial pressure, the pressure after the reaction increases as well. The temperature of the reaction products remains roughly the same. The velocity of gases in the nozzle decreases however. Case IV is particularily interesting, as the ignition did not occur for those initial conditions. A rapid increase in temperature, pressure and exit velocity can be observed, however these parameters then stabilize at their initial values. The spike is caused by injection of free hydrogen radicals. However the initial pressure proves to be too high for ignition to occur under these circumstances.

When initial temperature is increased, all of the parameters stay roughly the same. A small increase in exit velocity of gases and a small decrease of pressure of the reaction products can be observed.

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