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Computational Method in Combustion

Combustion in methane-oxygen rocket engine at various initial conditions

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Contents

1 Introduction

The goal of this paper is to demonstrate parameter changes of gas within the combustion chamber, as well as the products of combustion and the velocity of exhaust gases in relation to initial conditions. The mechanism used in this project is GRI-Mech 3, which is included in Cantera.

2 Theoretical model

The model used in the simulation process consists of seperate fuel and oxidizer tanks, from where the fuel and the oxidizer get to the combustion chamber, where they are burned. Combustion products escape through the nozzle. The simulation required creating a simplification of the whole process, which is represented by adopting the following assumptions:

- Fuel is injected in gas state,
- The combustion chamber is a zero-dimensional, reservoir
- Mass flow rate from the oxidizer and fuel tanks to the combustion chamber is constant,
- Flow through the nozzle is isentropic.

The stoichiometric reaction of complete combustion of propane in oxygen:

$$\mathrm{CH_4} + 202 \longrightarrow 2\,\mathrm{H_2O} + \mathrm{CO_2}$$

The simulation was performed for six different cases with varying initial conditions, stated below:

- I: Temperature: 300 K; Pressure in tanks: 10 atm,
- II: Temperature: 300 K; Pressure in tanks: 20 atm,
- III: Temperature: 300 K; Pressure in tanks: 40 atm,
- IV: Temperature: 800 K; Pressure in tanks: 20 atm,
- V: Temperature: 1200 K; Pressure in tanks: 20 atm;
- VI: Temperature: 1500 K; Pressure in tanks: 20 atm.

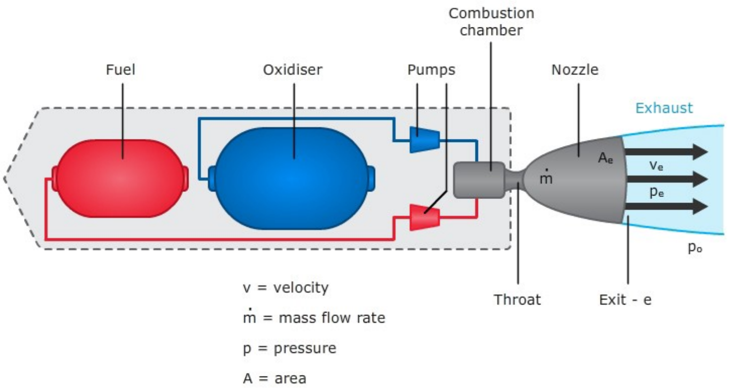


Figure 1: Simplified rocket engine scheme

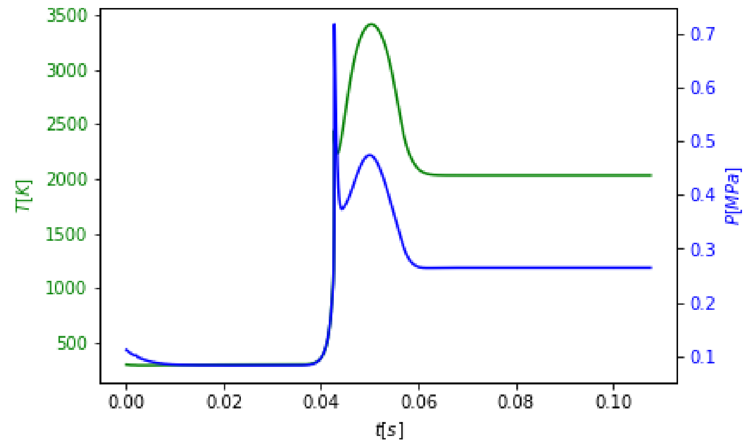
3 Code description

The project is based on calculations, using Python with the implementation of Cantera.
The beginning of the code mainly consists of creating reservoirs for fuel and oxidizer, as well as setting their initial temperature and pressure. Then, a combustion chamber and the ingition mechanism are created. The combustion chamber is 0,0005 square meters in volume and the ignition is caused by an injection of a small dose of free hydrogen radicals. Afterwards, there are functions, which calculate the 'kappa' coefficient. Knowing that the mass flow between reservoirs depends only on the area of the throat and after setting the following values:
$A_{CH4} = 4e^{-5}m^2$ - area of the methane injector
$A_{O2} = 4e^{-5}m^2$ - area of the oxygen injector
$A_{throat} = 1e^{-3}m^2$ - area of the nozzle's throat
It is possible to proceed to exhaust gas velocity calculations, using the equation below:

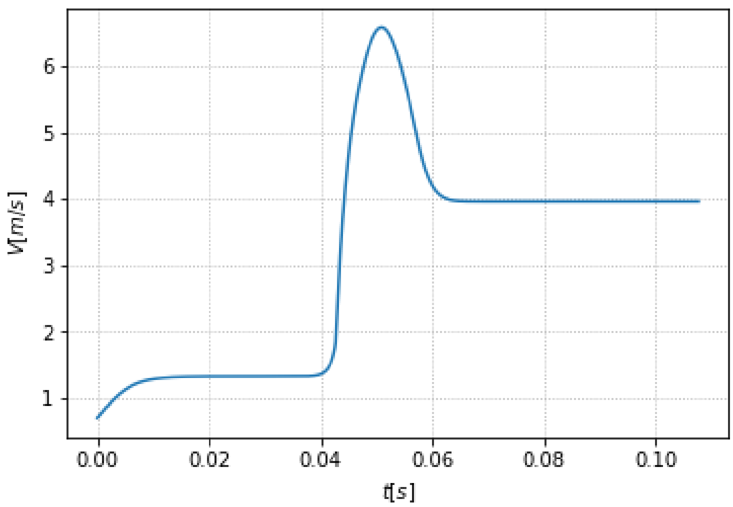
$$v_2 = \sqrt{2 * (kr/(k-1))T_0(1-(p_2/p-0)^{k-1/k})}$$

4 Results

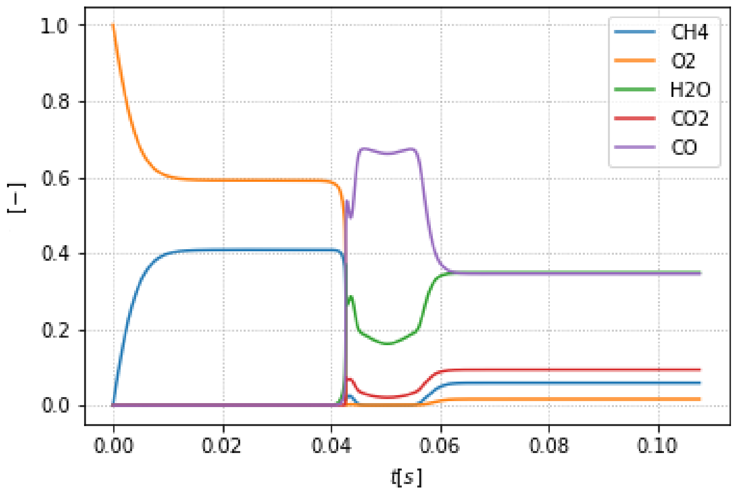
4.1 T=300K, p=10atm



Temperature and pressure in the combustion chamber

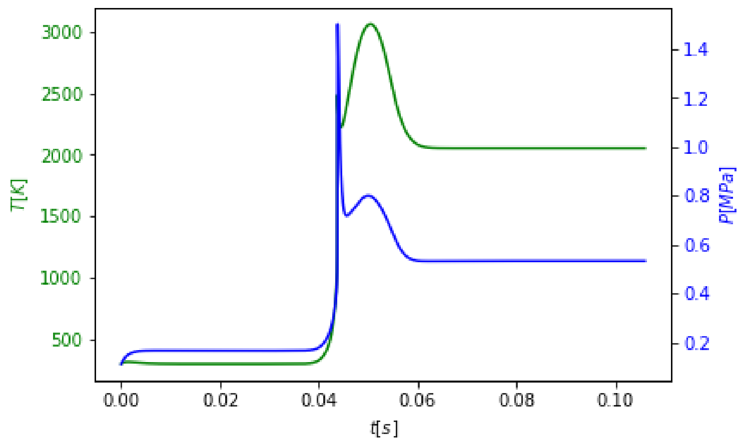


Velocity at the outlet of the nozzle

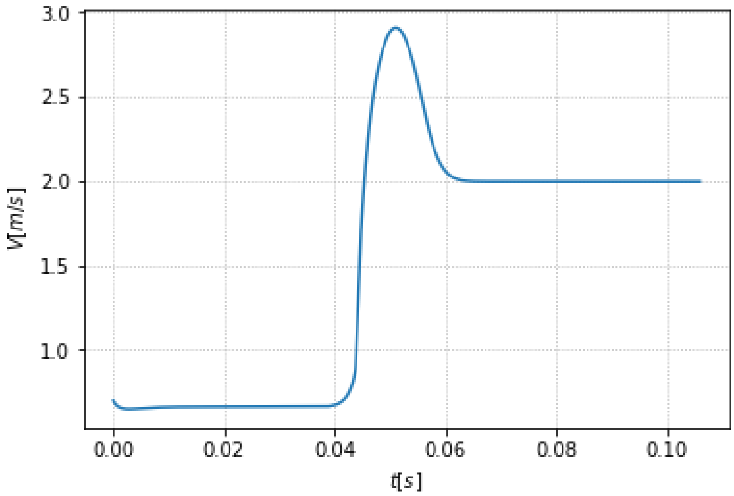


Masses of substrates and products

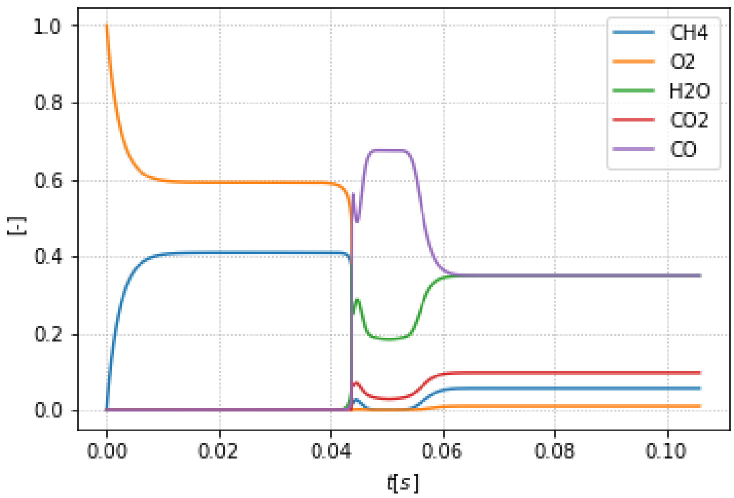
4.2 T=300K, p=20atm



Temperature and pressure in the combustion chamber

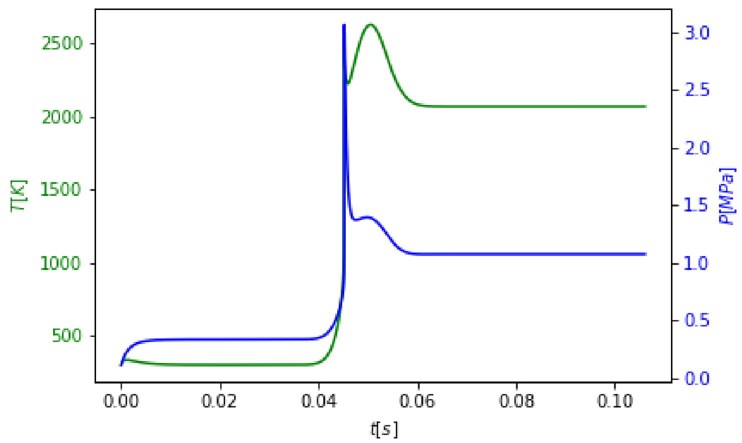


Velocity at the outlet of the nozzle

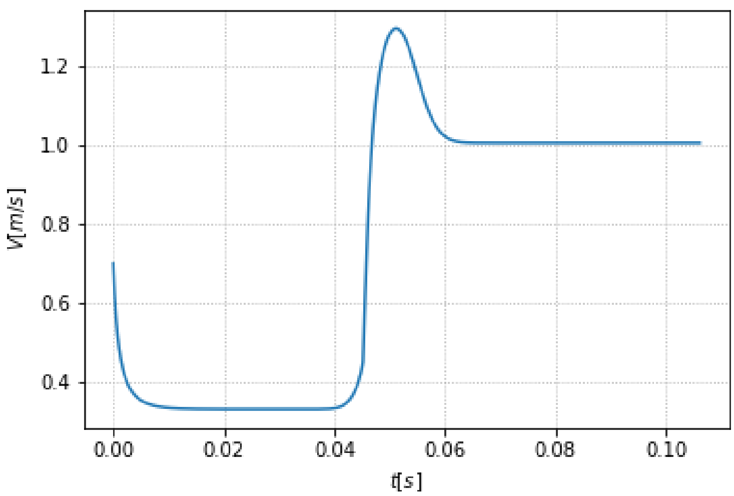


Masses of substrates and products

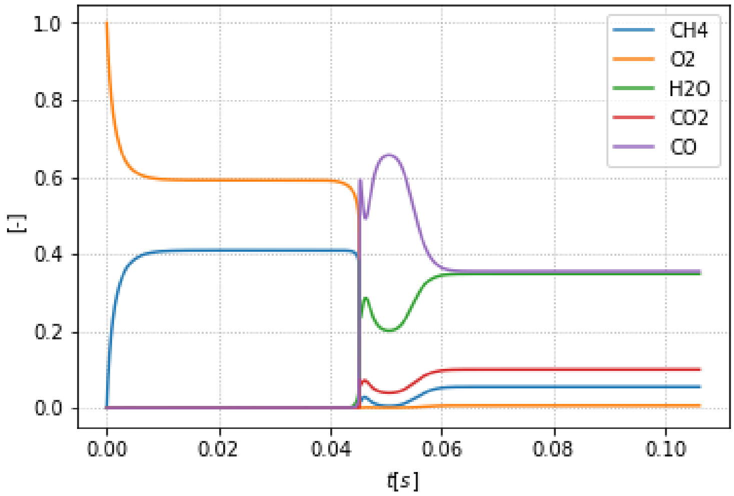
4.3 T=300K, p=40atm



Temperature and pressure in the combustion chamber

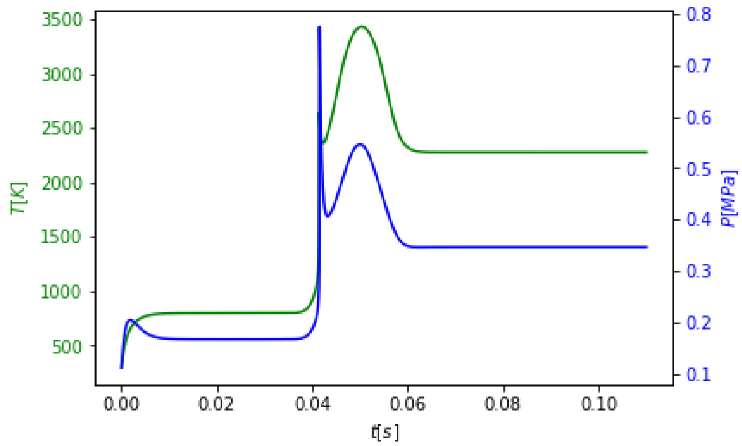


Velocity at the outlet of the nozzle

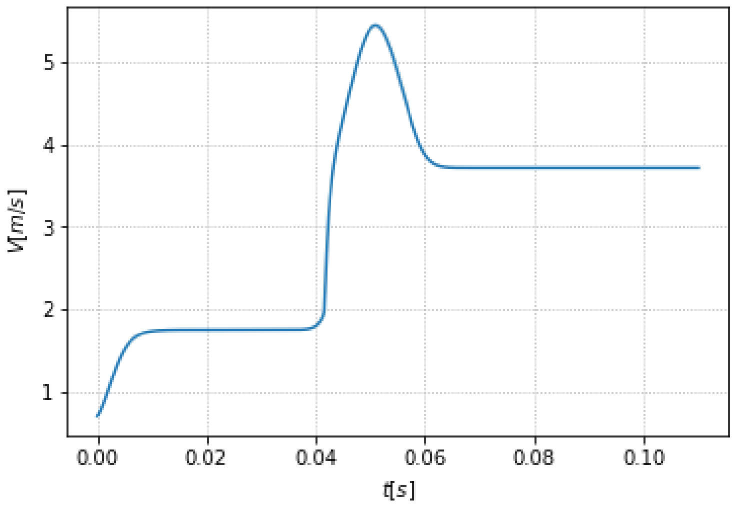


Masses of substrates and products

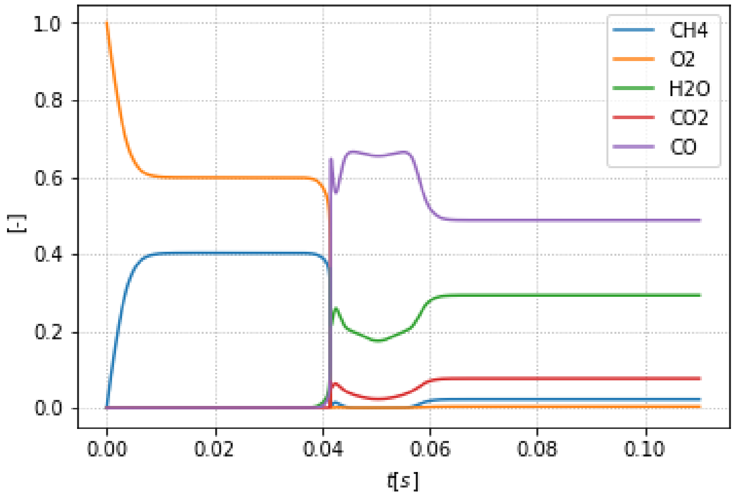
4.4 T=800K, p=20atm



Temperature and pressure in the combustion chamber

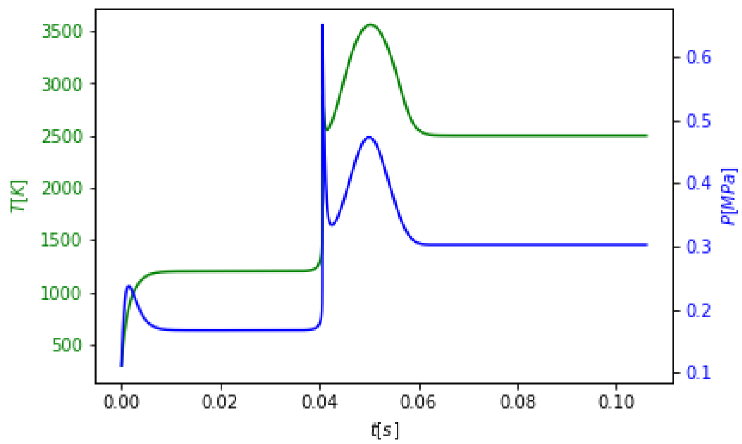


Velocity at the outlet of the nozzle

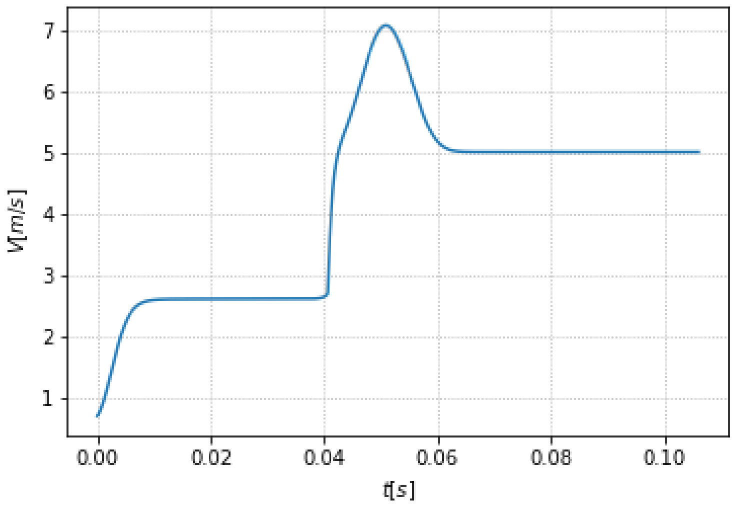


Masses of substrates and products

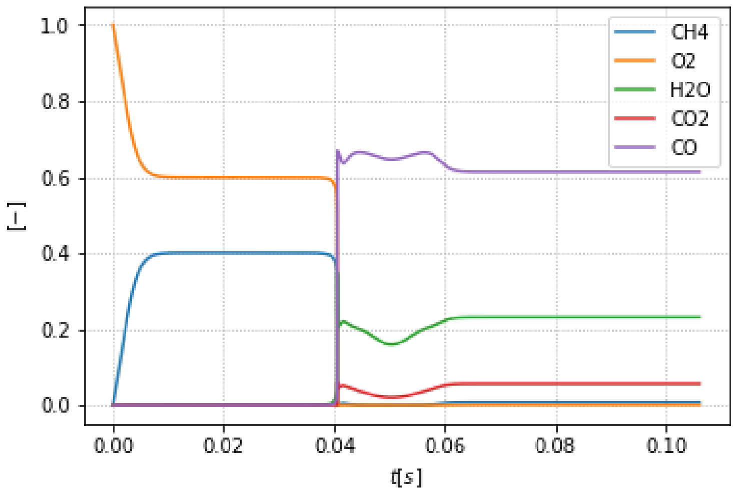
4.5 T=1200K, p=20atm



Temperature and pressure in the combustion chamber

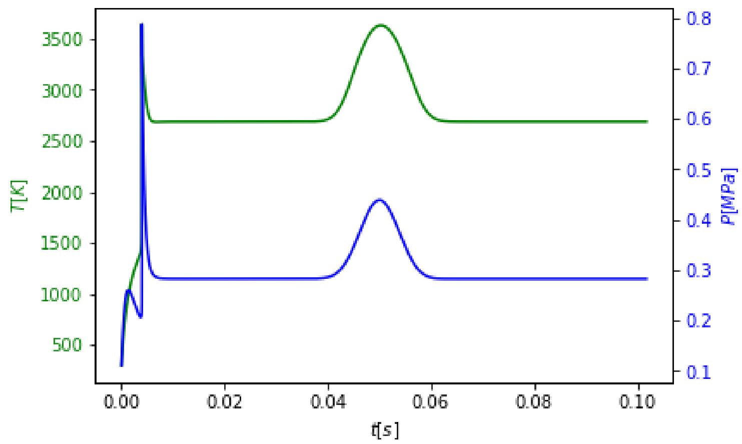


Velocity at the outlet of the nozzle

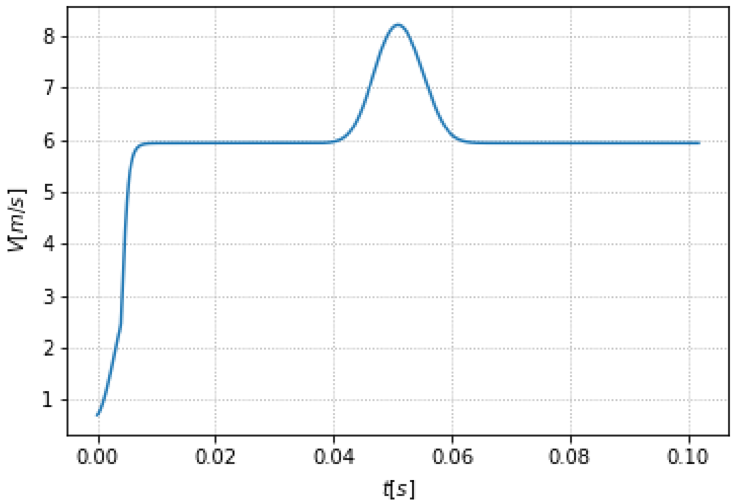


Masses of substrates and products

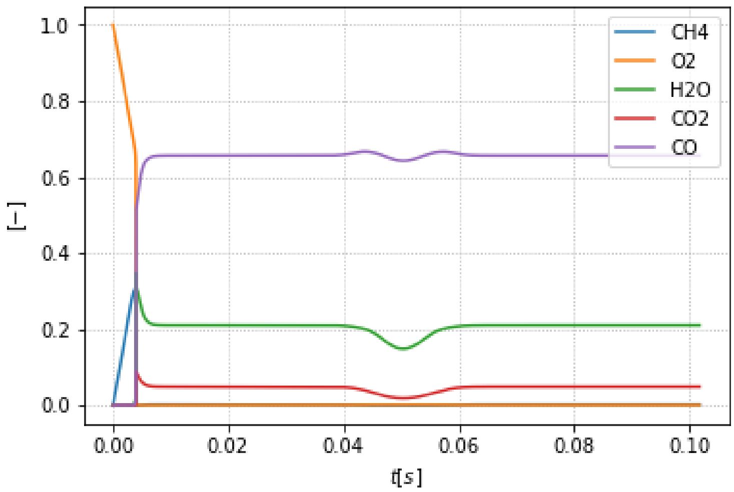
4.6 T=1500K, p=20atm



Temperature and pressure in the combustion chamber



Velocity at the outlet of the nozzle



Masses of substrates and products

5 Summary

Analysis of the results is leading to following conclusions:

- The higher the initial temperature within the fuel and oxidizer tanks, the higher the temperature in the combustion chamber, the higher the velocity at the end of the nozzle and the higher the amount of carbon monoxide within the products of the reaction.
- The higher the initial pressure in the fuel and oxidizer tanks, the higher the pressure in the combustion chamber, the lower the velocity at the end of the nozzle and the lower the amount of carbon monoxide within the products of the reaction.
- Peak of pressure at the 500 ms time mark represents the ignition.
- There are considerable amounts of methane and, as mentioned before, carbon monoxide within the products of the reaction, which points to the fact that partial combustion occurs.

6 References

[1] http://www.zamandayolculuk.com/html-2/roketdiagram.htm
[2] https://github.com/mranachowski/cantera_rocket_engine
[3] https://cantera.org/examples/python/reactors/combustor.py.html
[4] http://combustion.berkeley.edu/gri-mech/version30/text30.html