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Computational Methods in Combustion

Combustion in methane-oxygen rocket engine at various initial conditions

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1 Introduction

This paper aims to demonstrate parameter changes of gas within combustion chamber, the products of combustion and the velocity of exhaust in comparison to initial conditions. The mechanism used is the GRI-Mech 3 included in Cantera.

2 Theoretical model

The model used in the project consists of separate fuel and oxidizer tanks supplying ingredients that are to be burned in the combustion chamber. Combustion products escape through the nozzle. The project represents a simplified process compared to the real-life solution. The set conditions are:

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

The stoichiometric combustion of propane in oxygen:

$$CH_4 + 2O_2 \rightarrow 2H_2O + CO_2$$

The simulation was performed for six different varieties of initial conditions:

I – Temperature: 290 K; Pressure in the tanks: 15 atm;

II – Temperature: 290 K; Pressure in the tanks: 25 atm;

III – Temperature: 290 K; Pressure in the tanks: 35 atm;

IV – Temperature: 750 K; Pressure in the tanks: 25 atm;

V – Temperature: 1000 K; Pressure in the tanks: 25 atm;

VI – Temperature: 1300 K; Pressure in the tanks: 25 atm.

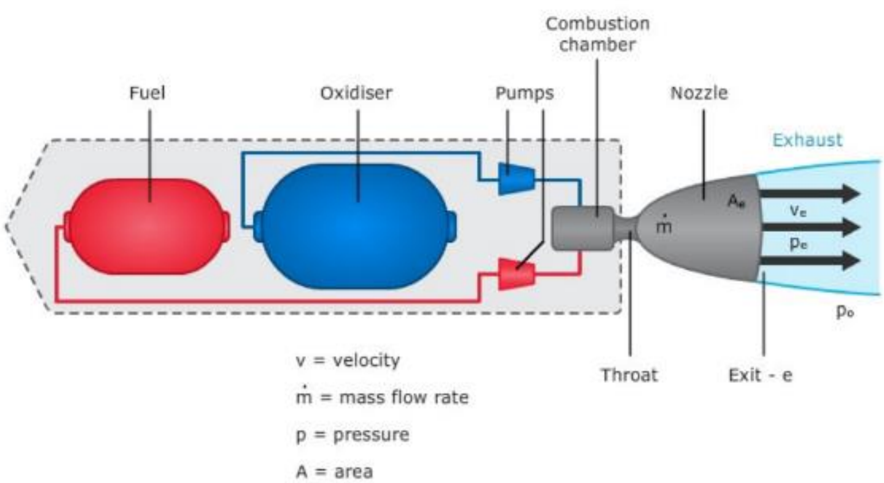


Figure 1: Simplified rocket engine scheme

3 Code description

The project is based on calculation using Python with implementation of Cantera. The initial part of the code consists of creating reservoirs for the fuel and the oxidizer and setting their parameters. Secondly, the combustion chamber and the ignition mechanism are created. The combustion chamber is 0,0005 sq. meters in volume and the ignition is started by an injection of a small dose of free hydrogen radicals. Furthermore, the “kappa” coefficient is calculated. 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 – are of the nozzle’s throat

It is possible to proceed to exhaust gas velocity calculations using the equation:

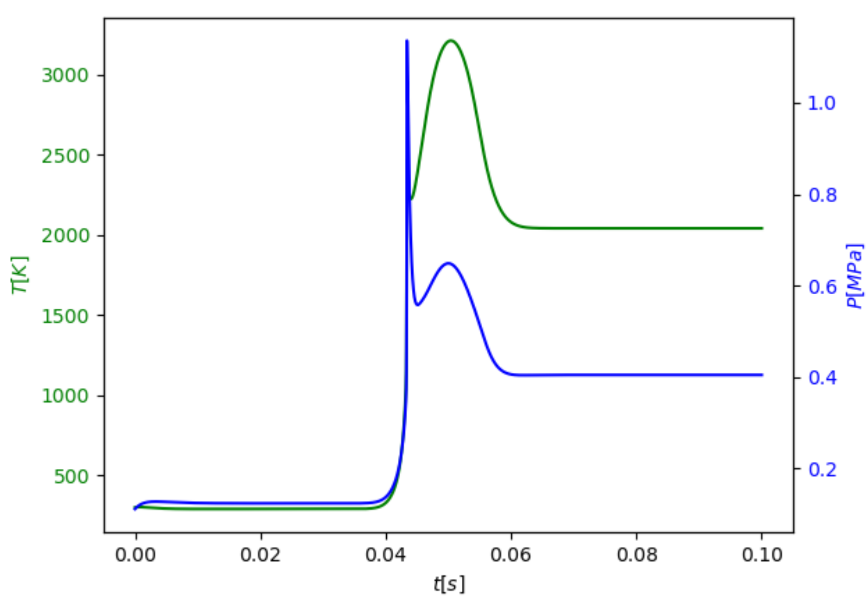
$$v_2 = \sqrt{2 * \left(\frac{kr}{k-1}\right) T0(1 - (\frac{p2}{p-p0})^{(k-1)/k}}$$

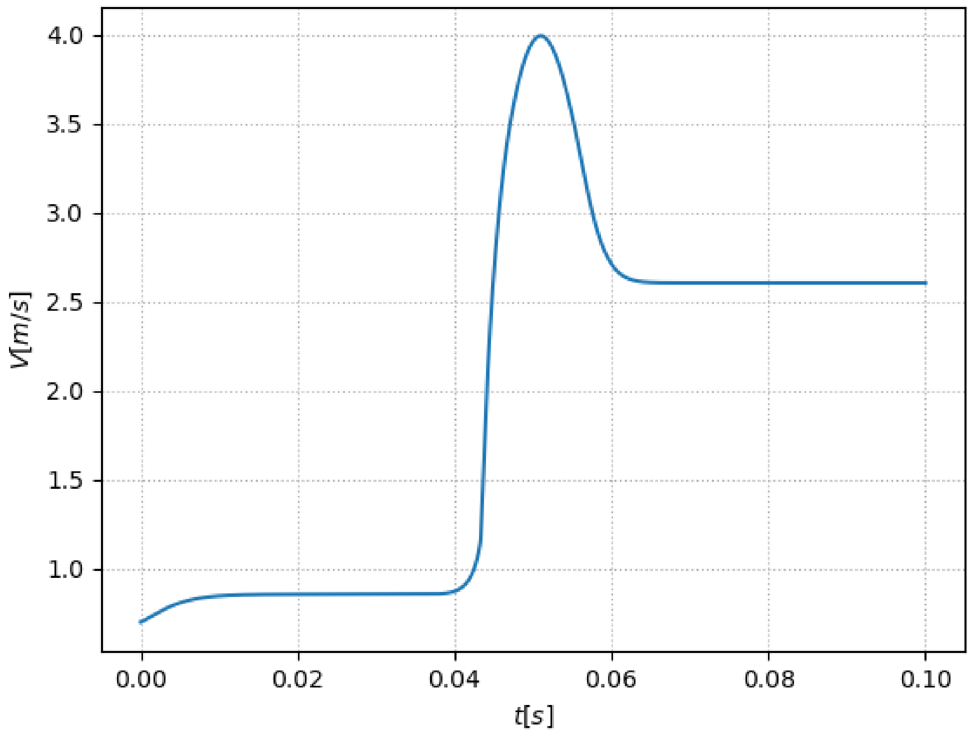
4 Results

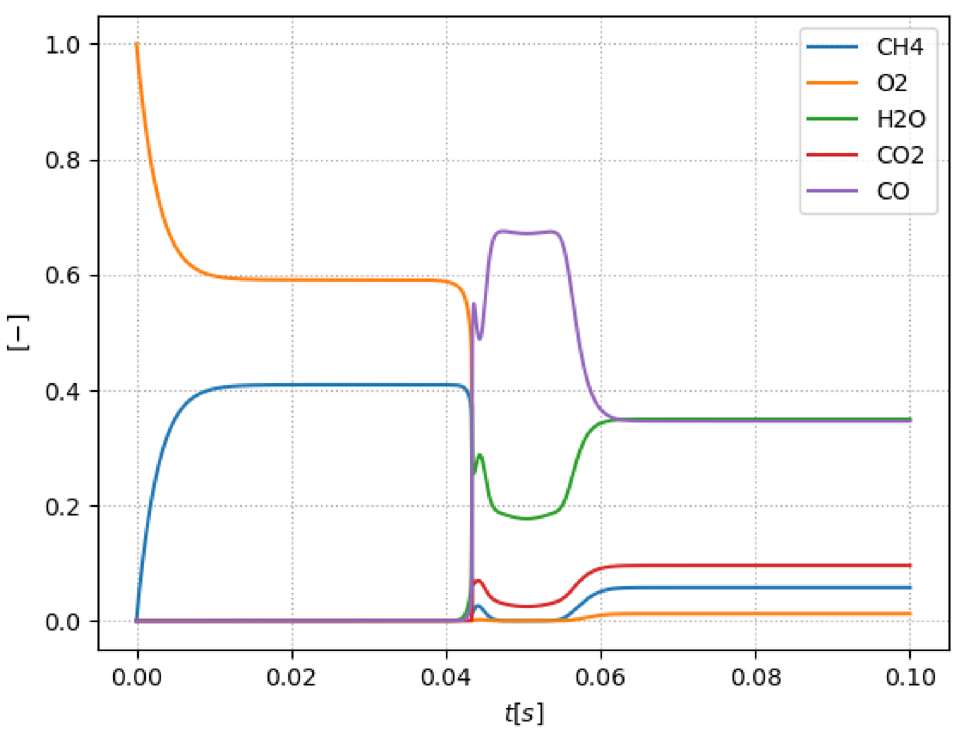
The graphs for particular cases are in that order:

- Temperature and pressure in combustion chamber
- Velocity at the outlet of the nozzle
- Masses of substrates and products

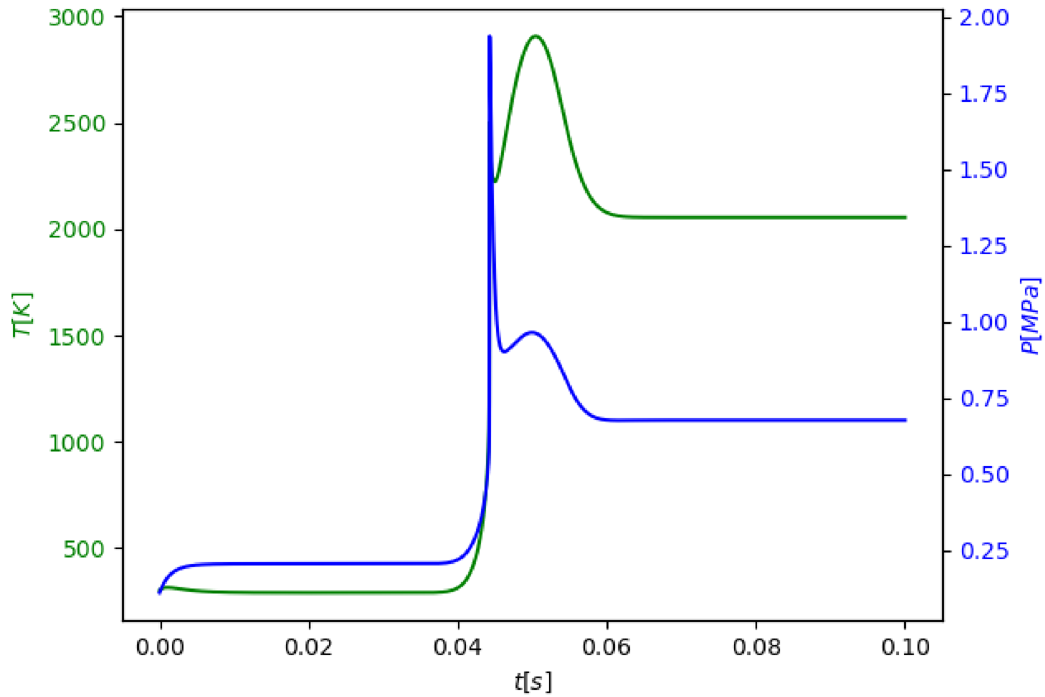
I – Temperature: 290 K; Pressure in the tanks: 15 atm

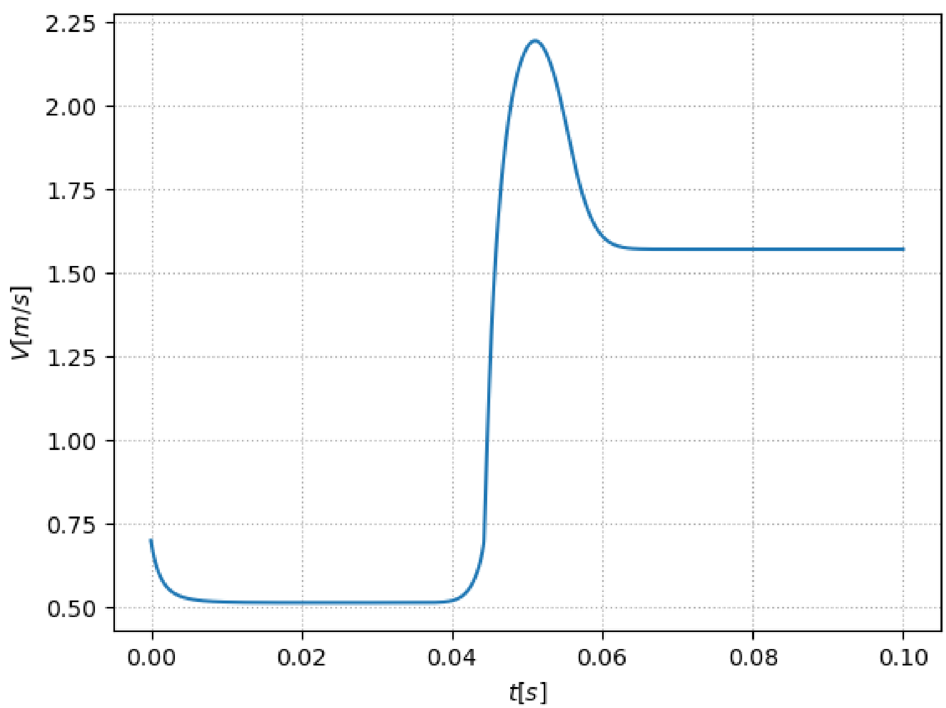


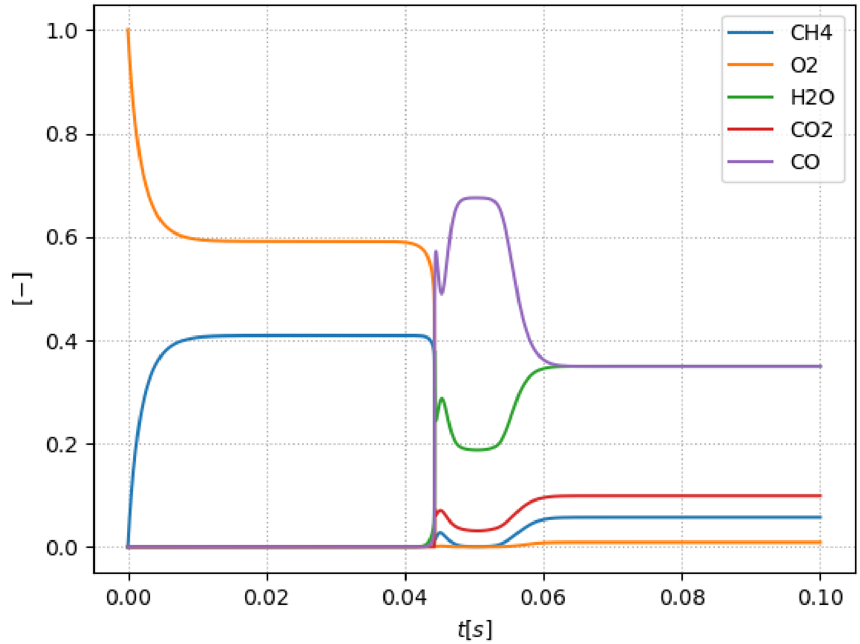

4.0
3.5
3.0
2.5
2.0
1.5
1.0
$V[m/s]$
0.00
0.02
0.04
0.06
0.08
0.10
$t[s]$


CH4
O2
H2O
CO2
CO
1.0
0.8
0.6
0.4
0.2
0.0
$[-]$
0.00
0.02
0.04
0.06
0.08
0.10
$t[s]$

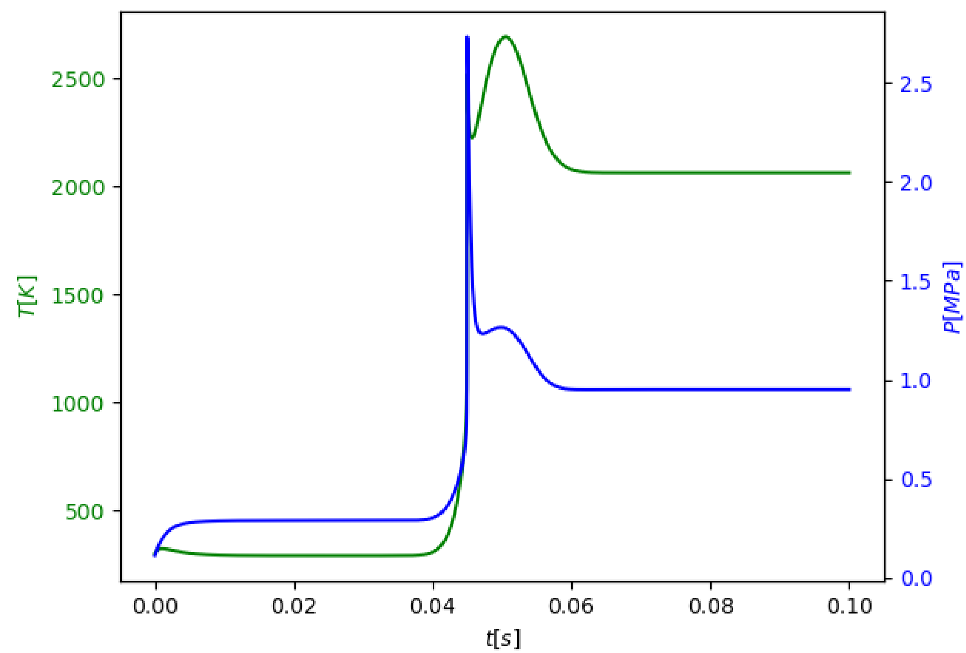
II – Temperature: 290 K; Pressure in the tanks: 25 atm

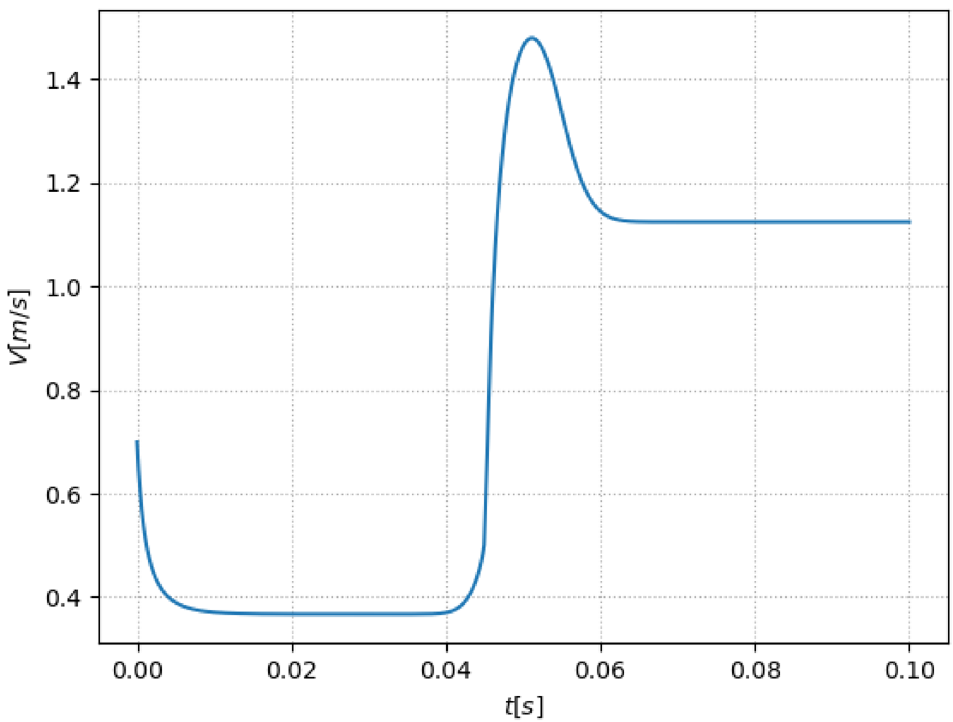


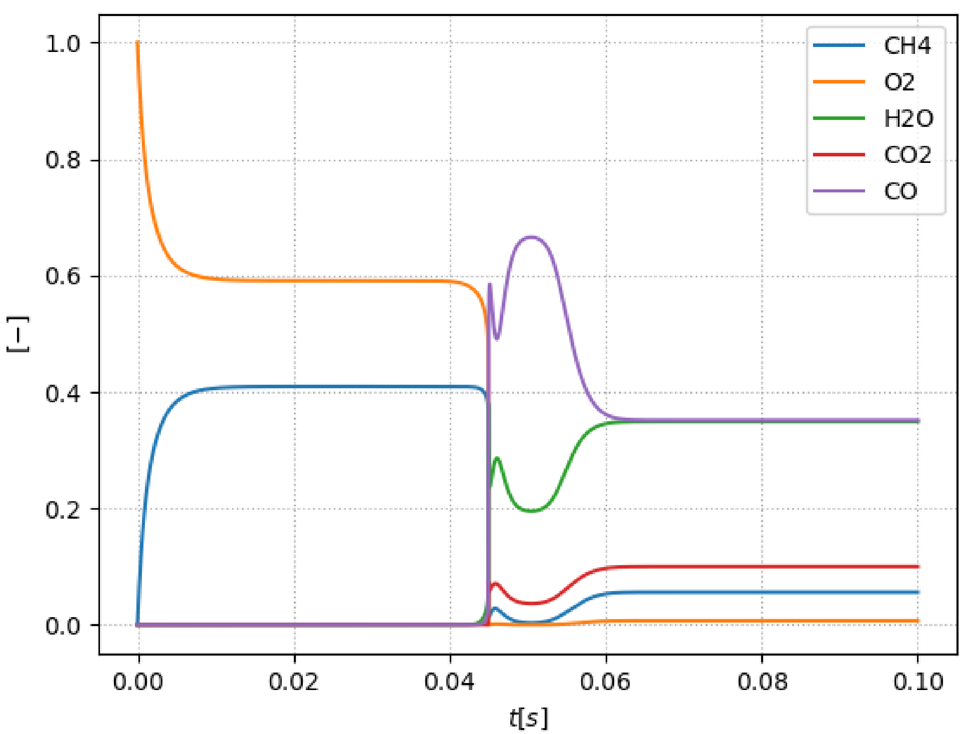




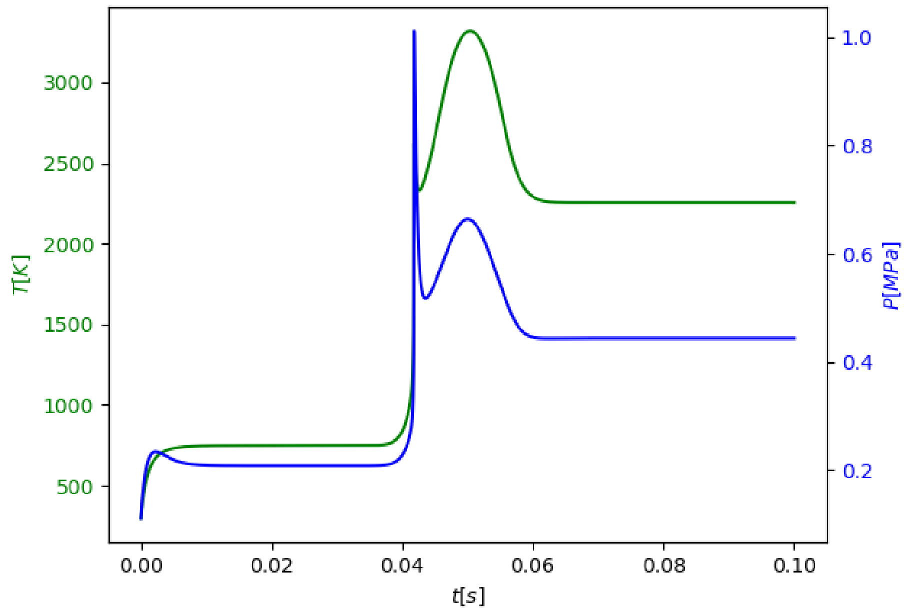
III – Temperature: 290 K; Pressure in the tanks: 35 atm

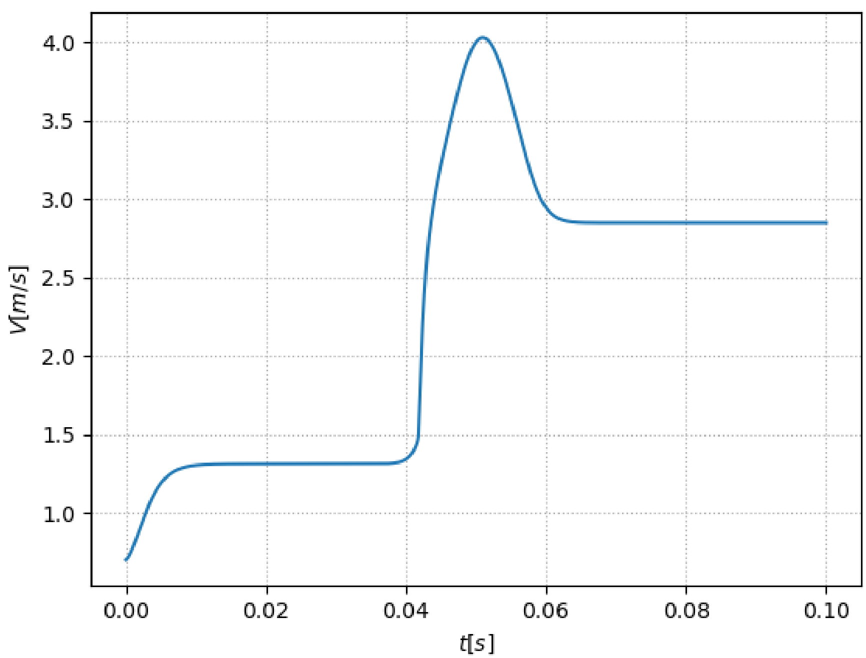


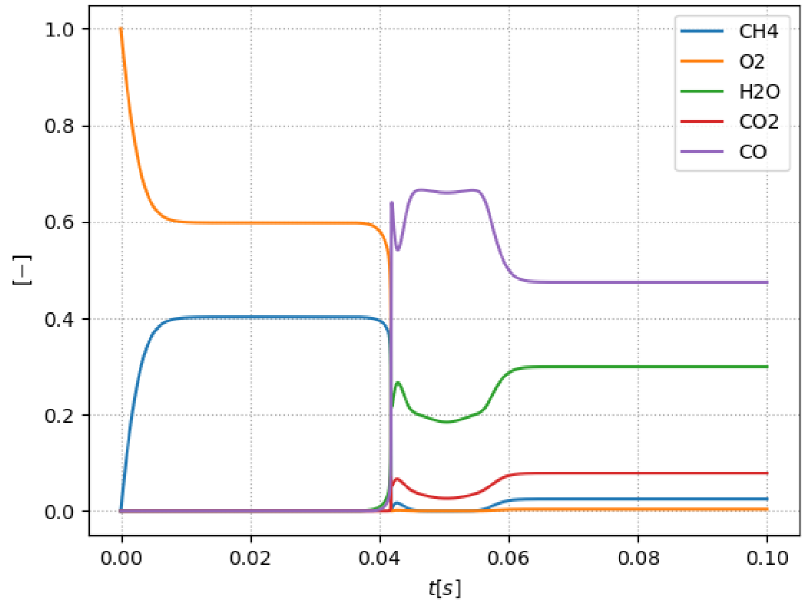

1.4
1.2
1.0
0.8
0.6
0.4
V[m/s]
0.00
0.02
0.04
0.06
0.08
0.10
t[s]


CH4
O2
H2O
CO2
CO
1.0
0.8
0.6
0.4
0.2
0.0
[−]
0.00
0.02
0.04
0.06
0.08
0.10
t[s]

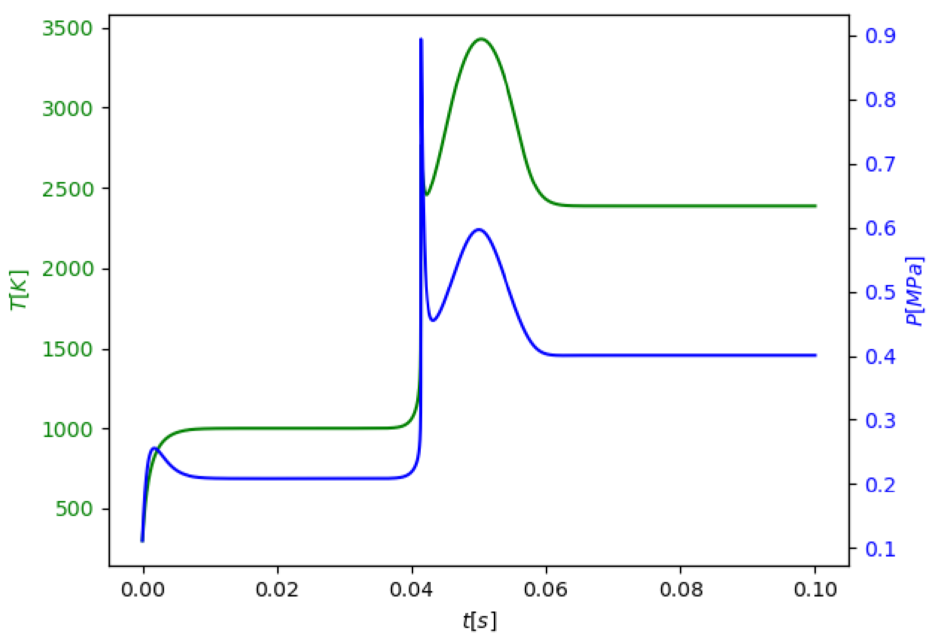
IV – Temperature: 750 K; Pressure in the tanks: 25 atm

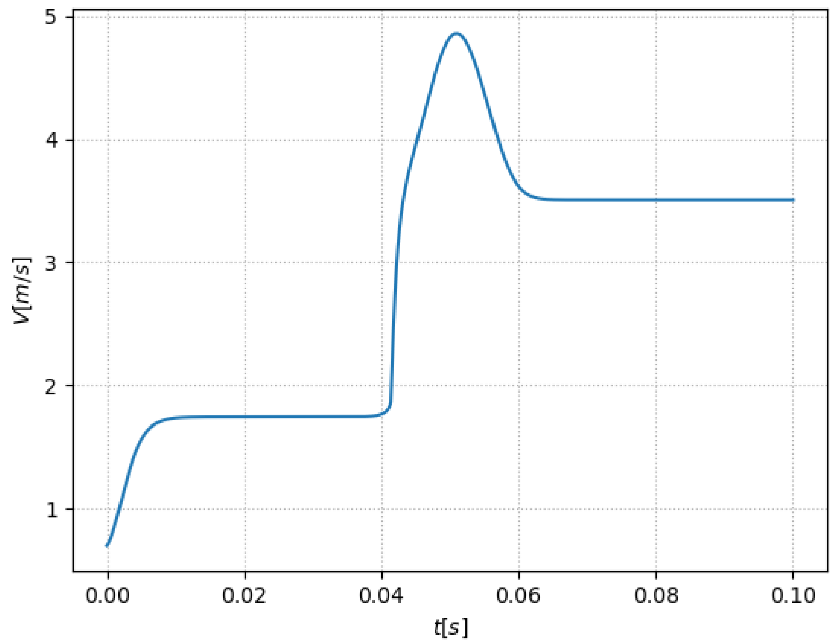




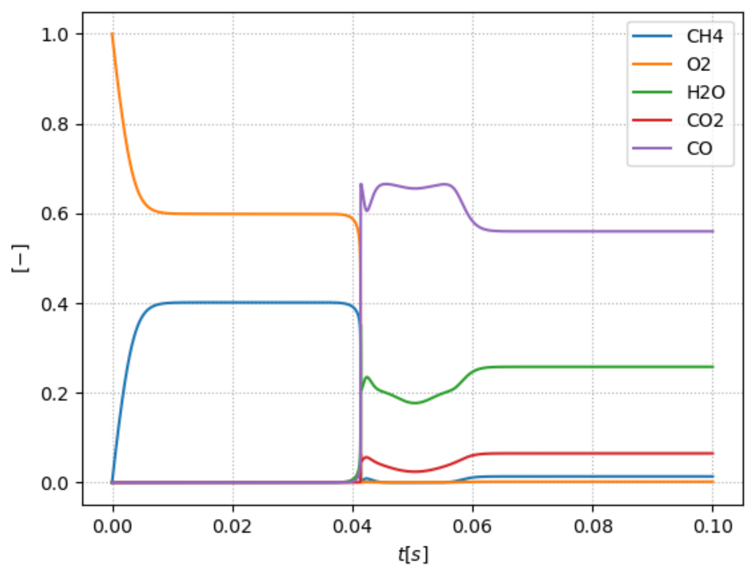


V – Temperature: 1000 K; Pressure in the tanks: 25 atm



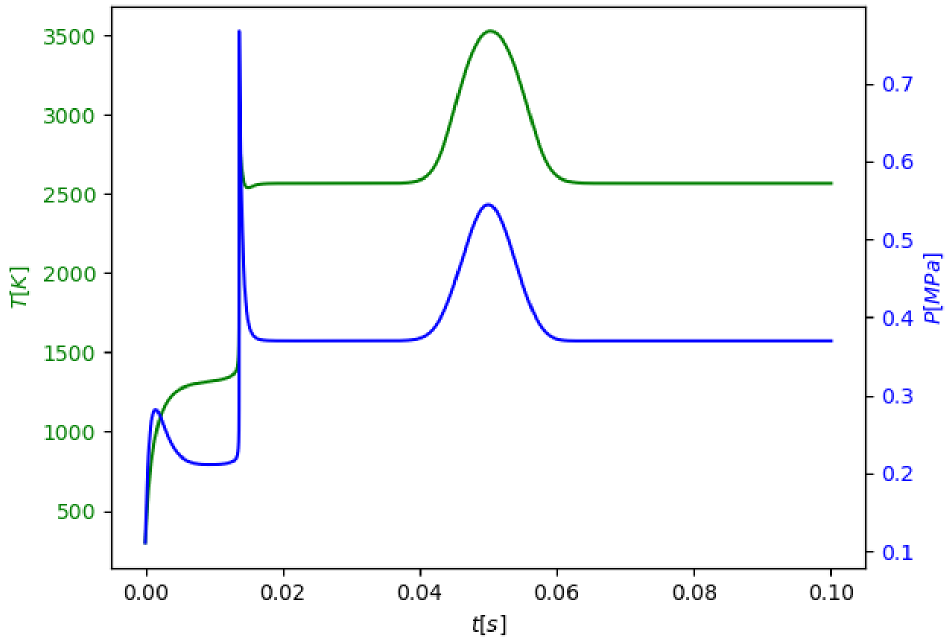


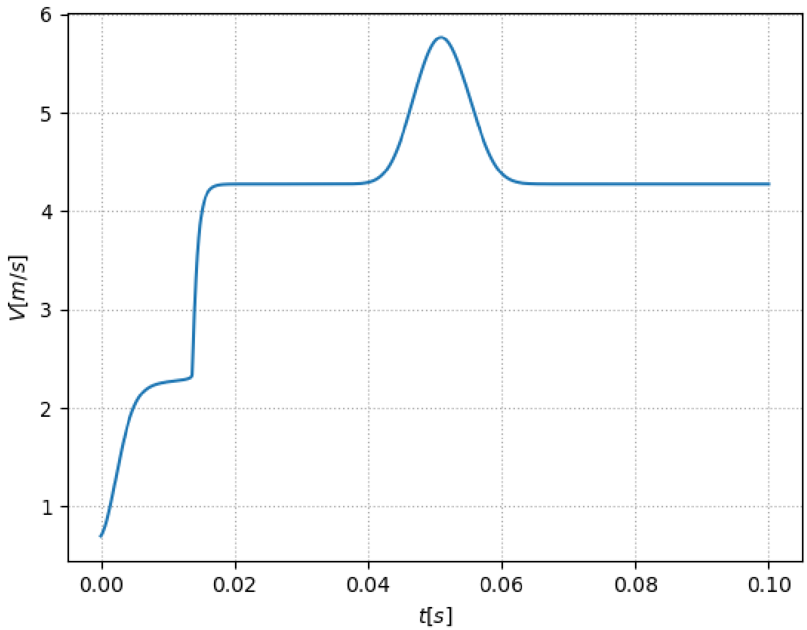
5
4
3
2
1
V[m/s]
0.00
0.02
0.04
0.06
0.08
0.10
t[s]

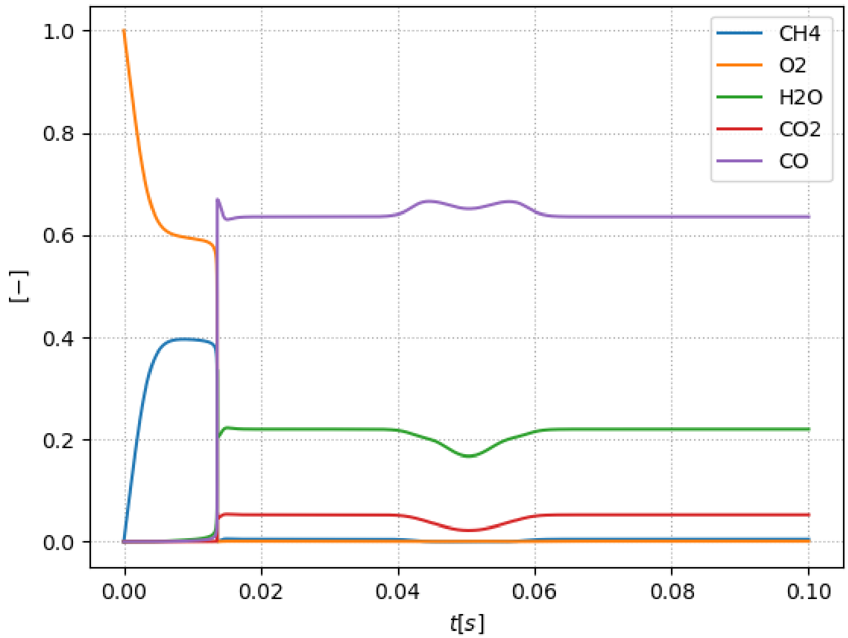


CH4
O2
H2O
CO2
CO
1.0
0.8
0.6
0.4
0.2
0.0
[−]
0.00
0.02
0.04
0.06
0.08
0.10
t[s]

VI – Temperature: 1300 K; Pressure in the tanks: 25 atm







5 Summary

-The higher the initial temperature within the fuel and oxidizer tanks the higher the temperature in the combustion chamber. Higher velocity at the end of the nozzle is generated and more carbon monoxide is created as a product od reaction.

-The higher the initial pressure in the fuel ad oxidizer tanks the higher the pressure in the combustion chamber. Lower velocity is generated at the end of the nozzle and less carbon monoxide is created.

-Peak of pressure represents time of ignition.

- Considering the amount of methane and carbon monoxide post-combustion it is safe to assume 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