The Faculty of Power and Aeronautical Engineering
Warsaw University of Technology

Computational Methods in Combustion

Combustion in methane-oxygen rocket engine at various initial conditions

Jakub Bochocki

Warsaw 2024

Contents

Introduction

This paper aims to demonstrate how gas parameters within the combustion chamber, the combustion products, and the velocity of exhaust gases vary in relation to initial conditions. The project utilizes the GRI-Mech 3 mechanism, which is integrated into Cantera.

Theoretical model

The simulation model comprises separate fuel and oxidizer tanks that supply the combustion chamber, where combustion occurs. The resulting combustion products are expelled through a nozzle. To facilitate the simulation, the process was simplified 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 methane in oxygen:

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

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

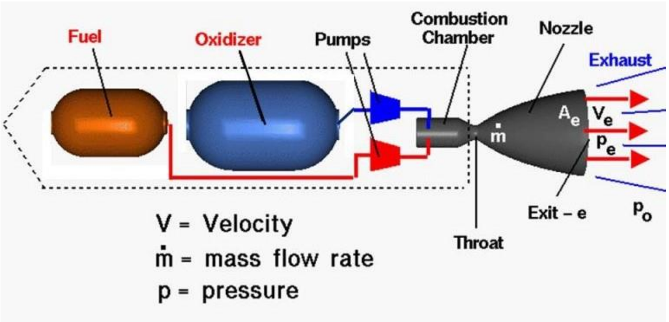
I: Temperature T = 293K (20°C), pressure p = 20 atm;

II: Temperature T = 293K (20°C), pressure p = 30 atm;

III: Temperature T = 293K (20°C), pressure p = 40 atm;

IV: Temperature T = 773K (500°C), pressure p = 20 atm;

V: Temperature T = 1273K (1000°C), pressure p = 20 atm;



Program structure

The initial part of the code focuses on creating reservoirs for the fuel and oxidizer and setting their initial temperatures and pressures. Following this, a combustion chamber and an ignition mechanism are established. The combustion chamber has a volume of 0.0005 square meters, and ignition is achieved by injecting a small dose of free hydrogen radicals. Afterwards, functions are implemented to calculate the adiabatic exponent κ and valve coefficient. This function is based on critical flow in nozzle. In consequence the mass flow between reservoirs depends only on area of injector/throat.

$A_{CH_4} = 4e^{-5}\ m^2$ – area of methane injector;

$A_{O_2} = 4e^{-5}\ m^2$ – area of oxygen injector;

$A_{throat} = 1e^{-3}\ m^2$ – area of nozzle's throat;

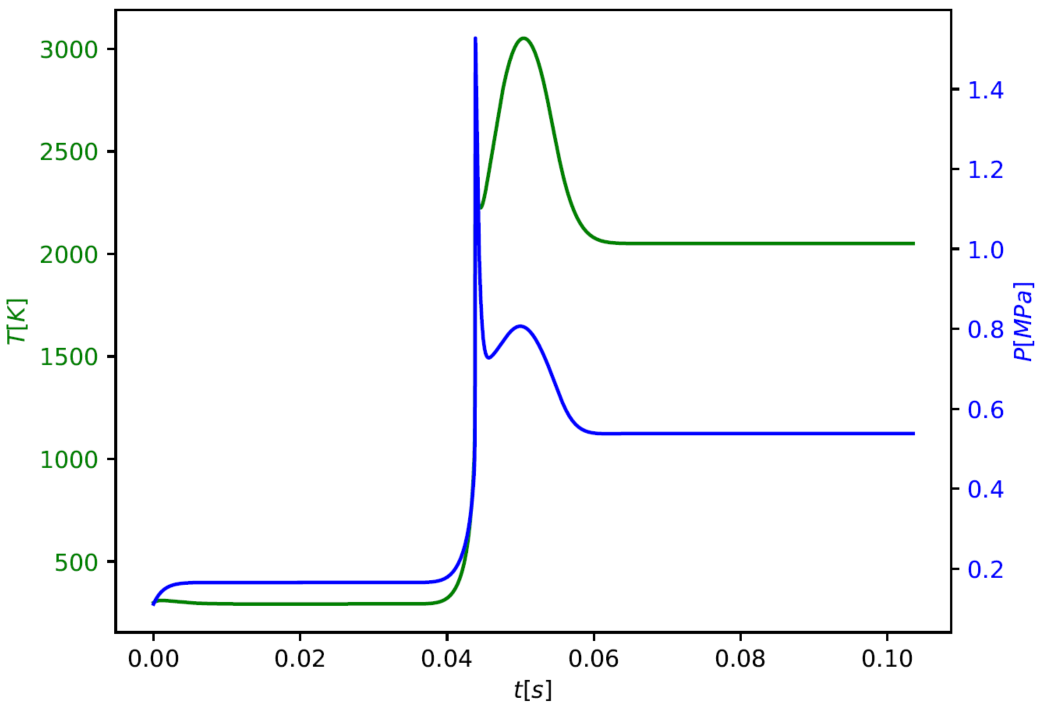
The velocity of exhaust gases can be calculated using formula:

$$v_e = \sqrt{2 * \frac{\kappa R}{\kappa - 1} T * (1 - (\frac{p_e}{p - 0})^{\frac{\kappa - 1}{\kappa}})}$$

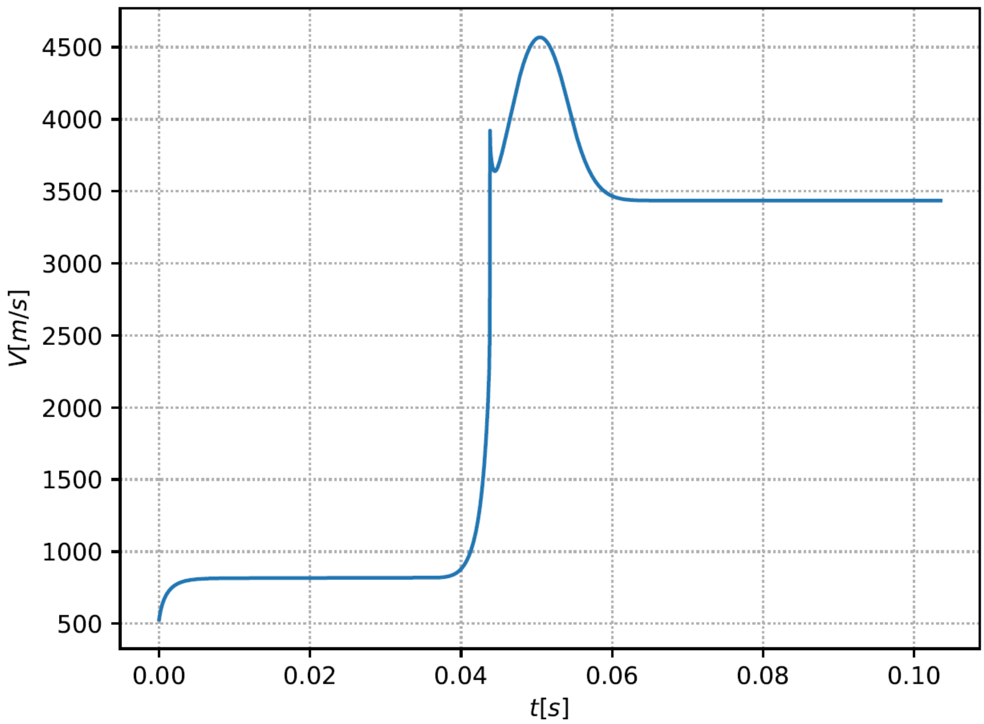
Results

Temperature T = 293K (20°C), pressure p = 20 atm:

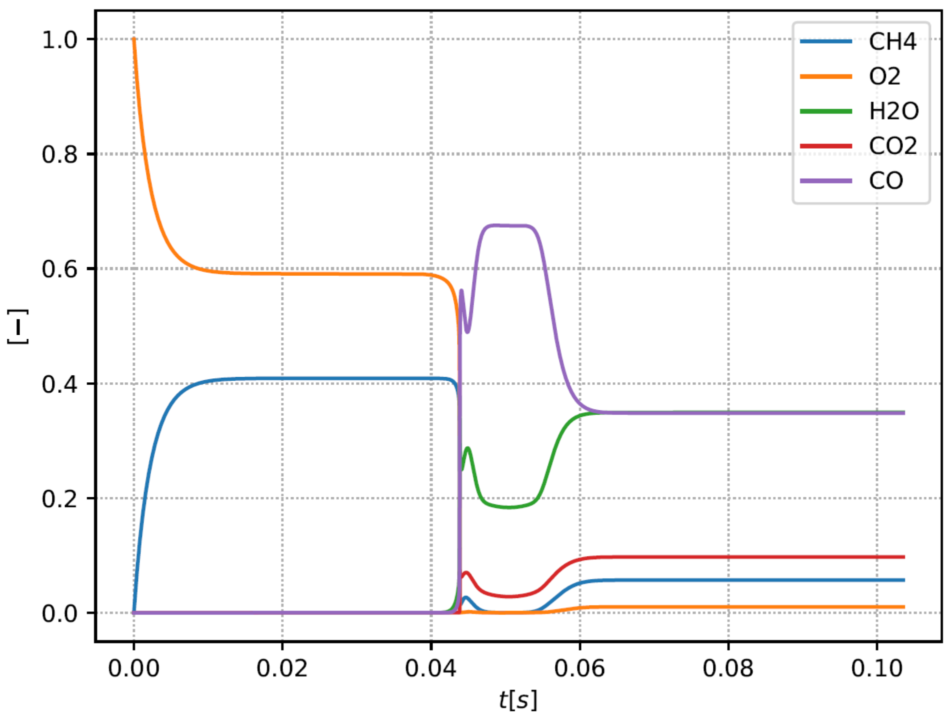
Temperature and pressure in the combustion chamber:



Velocity at the outlet of the nozzle:

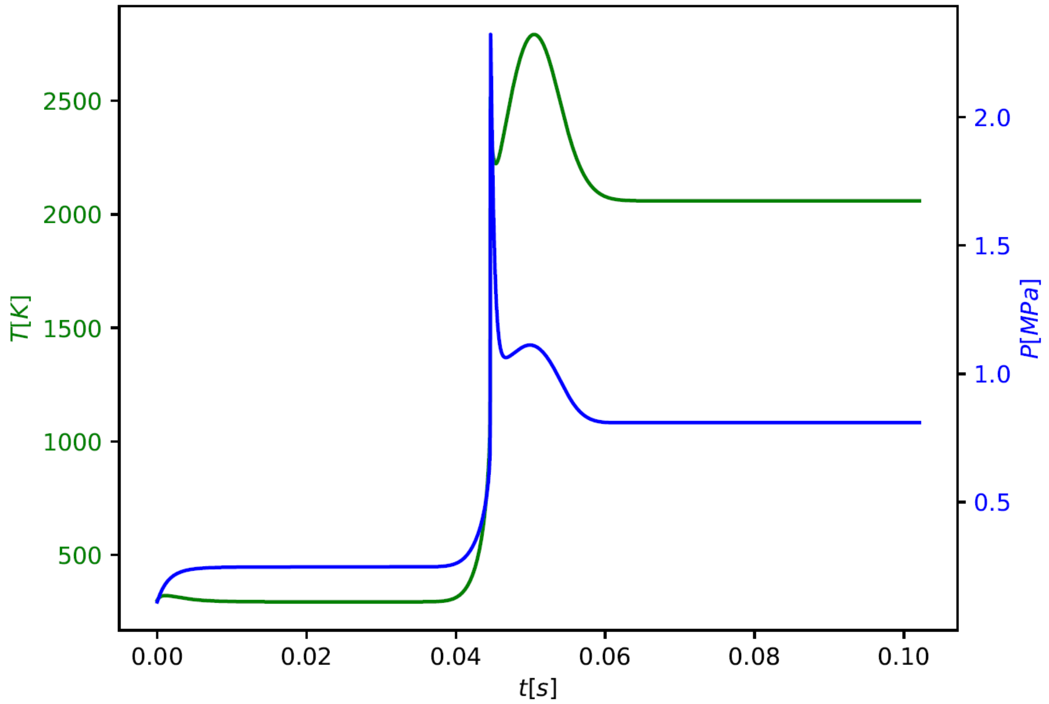


Masses of substrates and products in the combustion chamber:

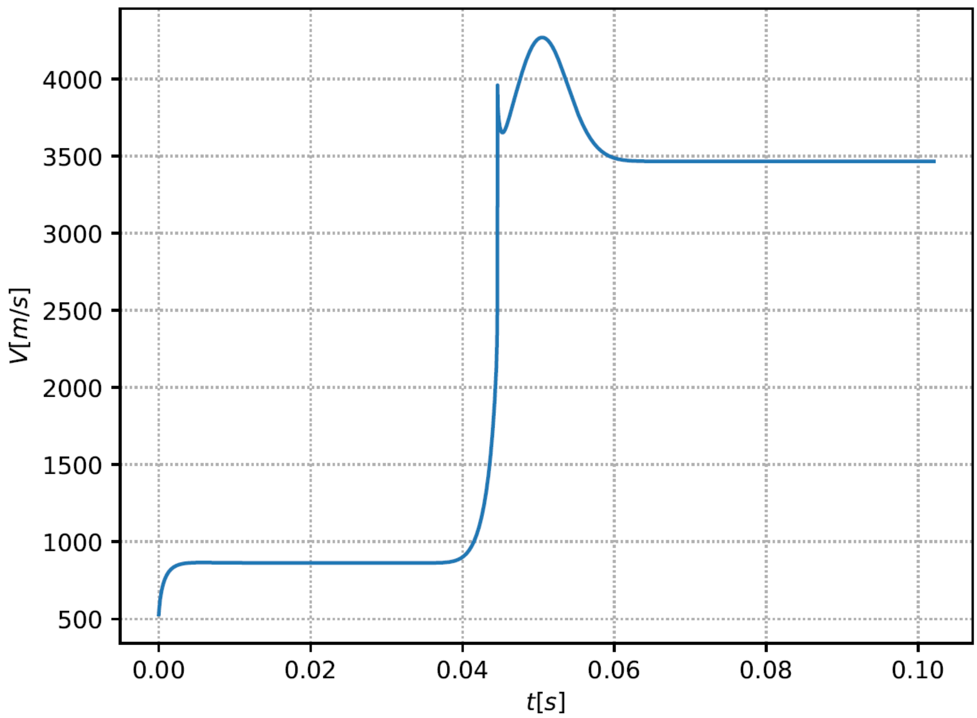


Temperature T = 293K (20°C), pressure p = 30 atm:

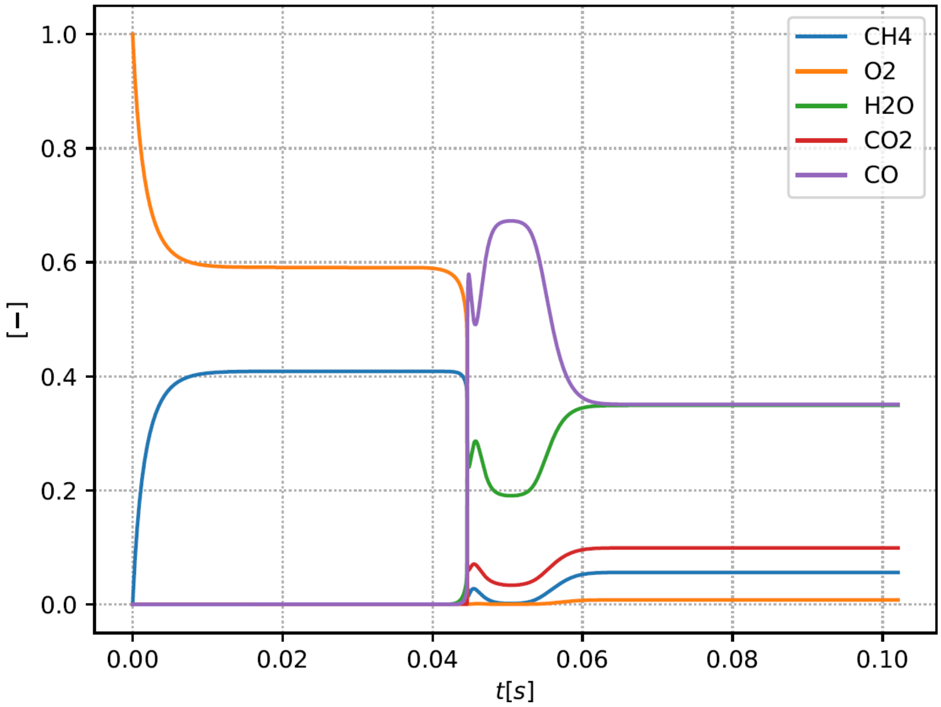
Temperature and pressure in the combustion chamber:



Velocity at the outlet of the nozzle:

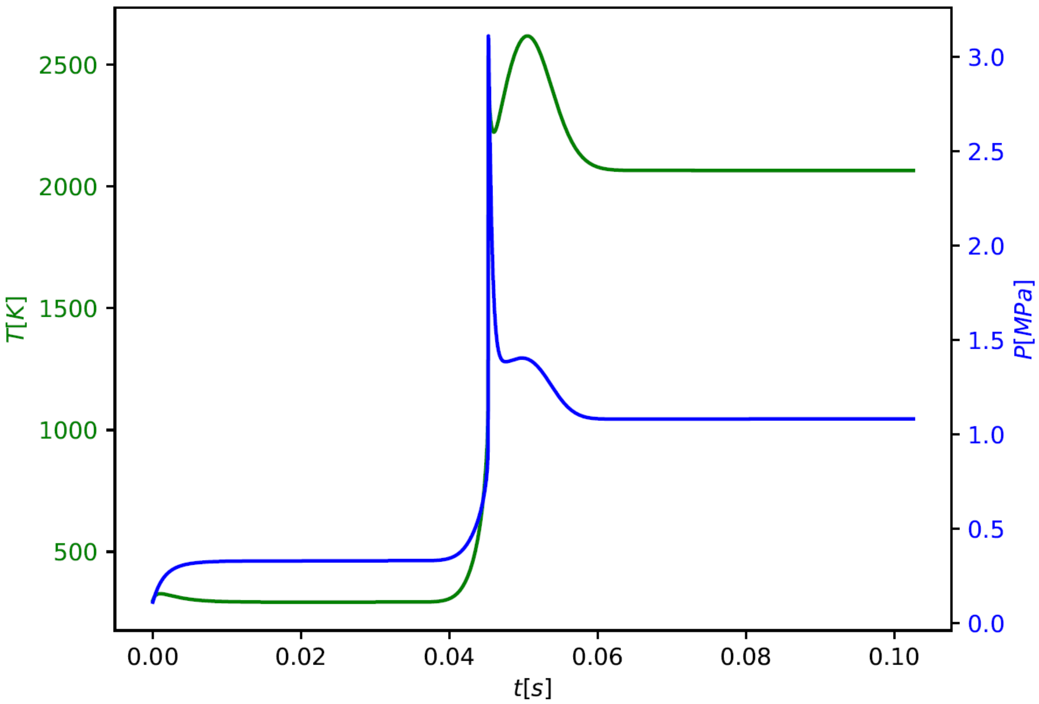


Masses of substrates and products in the combustion chamber:

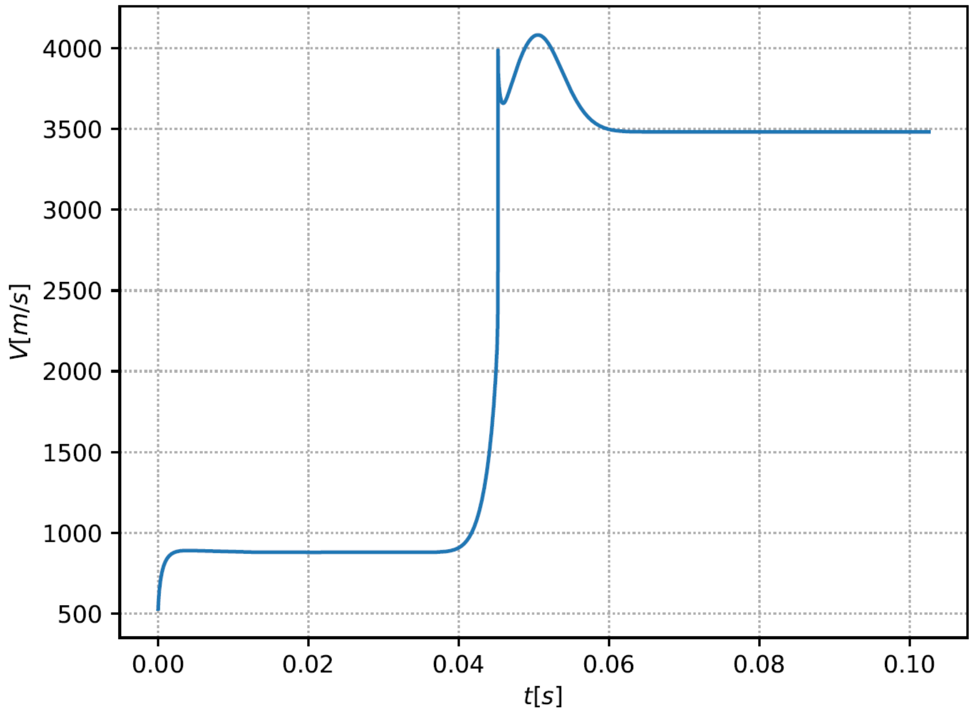


Temperature T = 293K (20°C), pressure p = 40 atm:

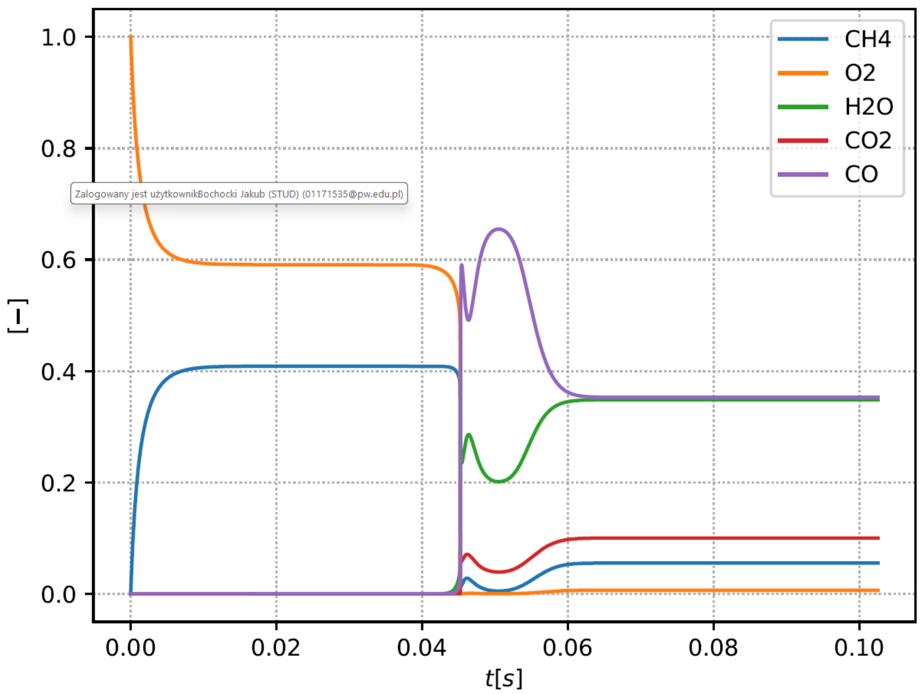
Temperature and pressure in the combustion chamber:



Velocity at the outlet of the nozzle:

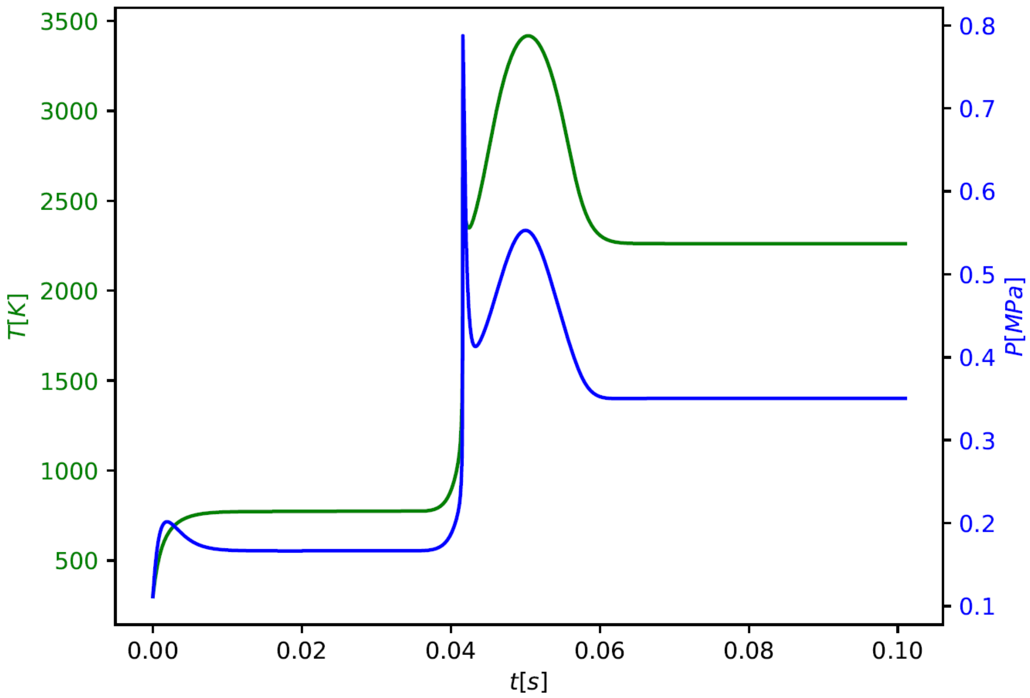


Masses of substrates and products in the combustion chamber:

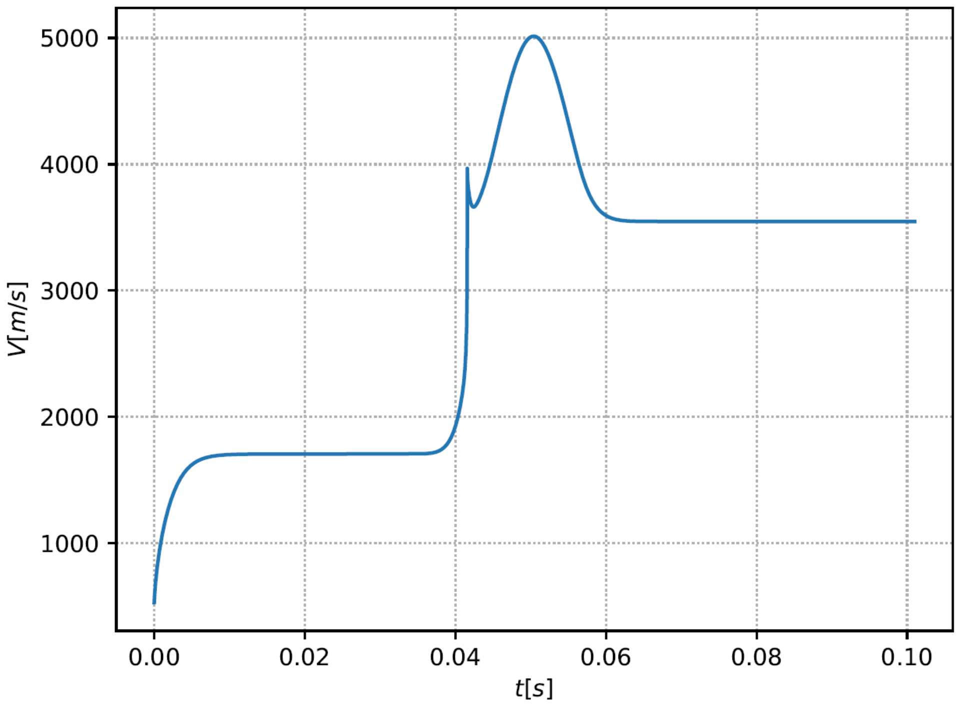


Temperature T = 773K (500°C), pressure p = 20 atm:

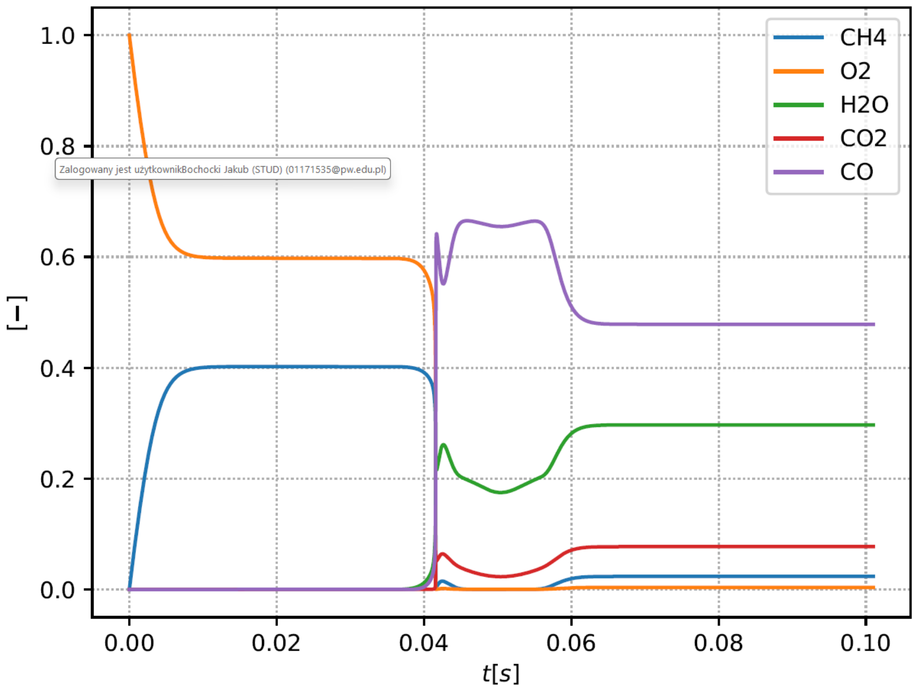
Temperature and pressure in the combustion chamber:



Velocity at the outlet of the nozzle:

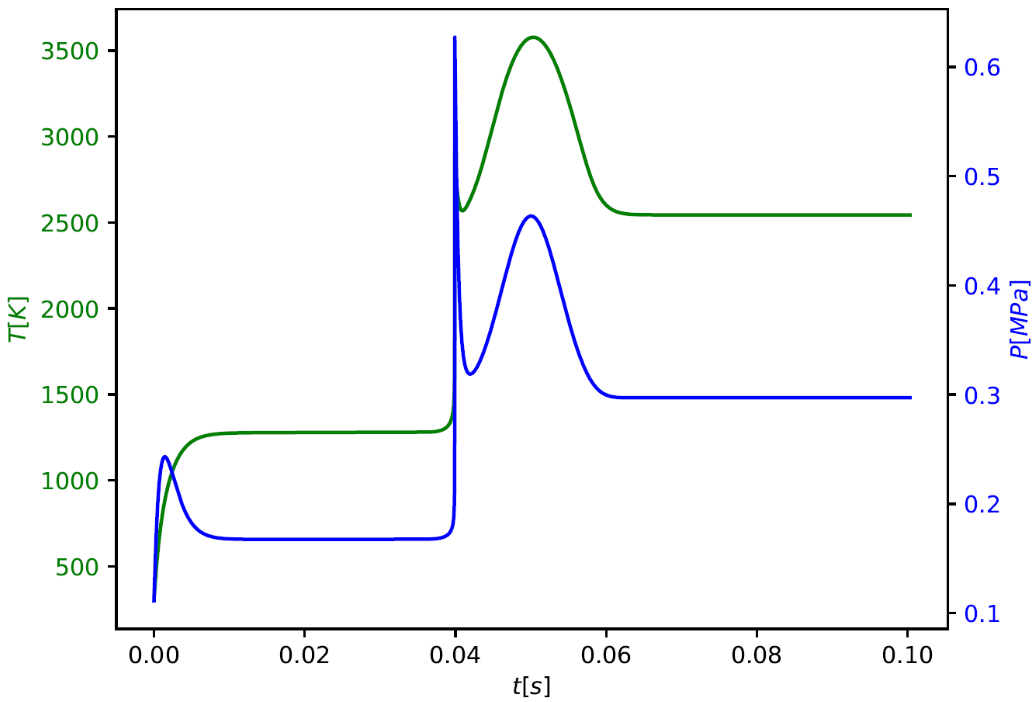


Masses of substrates and products in the combustion chamber:

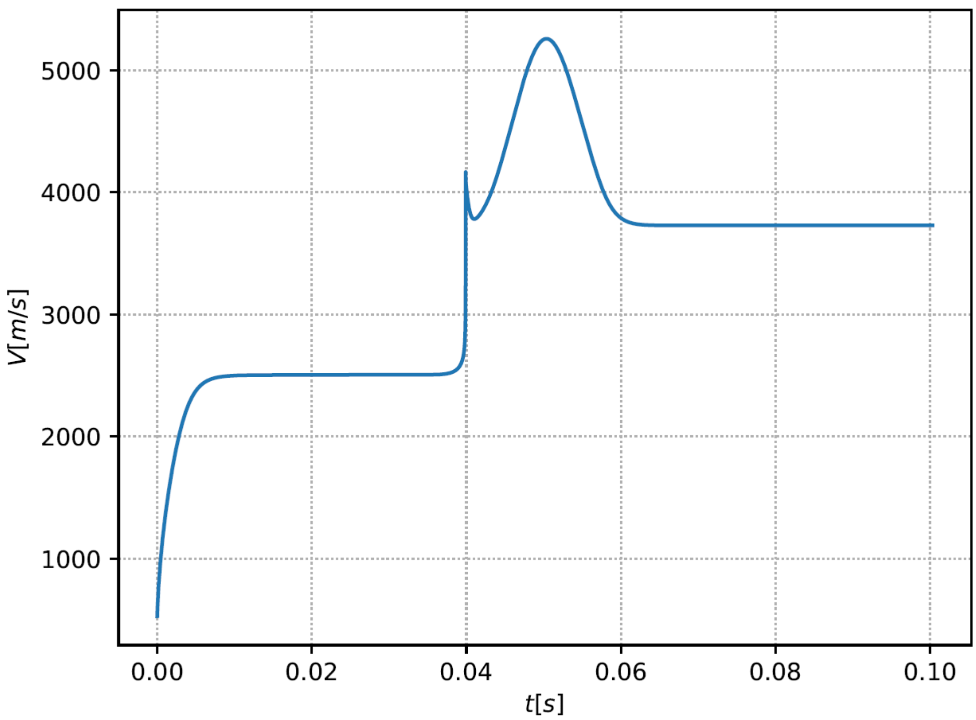


Temperature T = 1273K (1000°C), pressure p = 20 atm:

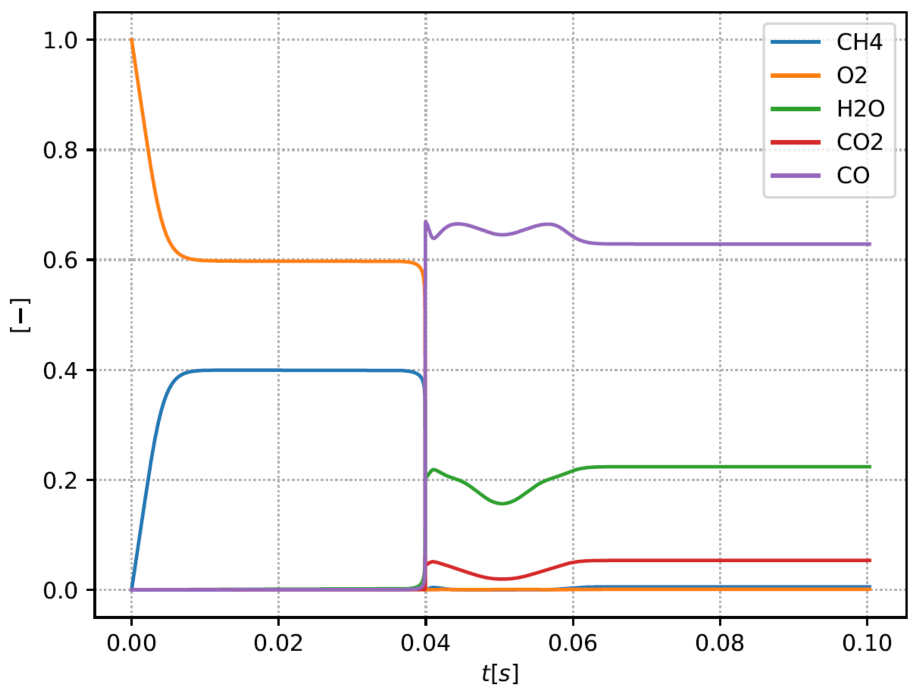
Temperature and pressure in the combustion chamber:



Velocity at the outlet of the nozzle:



Masses of substrates and products in the combustion chamber:



Summary

- The initial temperature in the fuel and oxidizer tanks directly affects the combustion process: higher initial temperatures lead to higher temperatures in the combustion chamber, increased exhaust gas velocity at the nozzle exit, and greater amounts of carbon monoxide in the reaction products.
- Higher initial pressure in the fuel and oxidizer tanks results in increased pressure in the combustion chamber and reduced velocity at the nozzle exit.
- Peak of pressure at the 500 ms time mark represents the ignition.
- Significant amounts of methane and carbon monoxide are present in the reaction products, indicating that partial combustion has occurred.

References

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