The Faculty of Power and Aeronautical Engineering Warsaw University of Technology



Computational Method in Combustion

Combustion in ethane-oxygen rocket engine at various initial conditions

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1 Introduction

The goal of this paper is to demonstrate how gas' parameter changes in 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 separate 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 stechiometric reaction of complete combustion of ethane in oxygen

$$\mathrm{C_2H_6} + \tfrac{7}{2}\mathrm{O_2} \longrightarrow 3\,\mathrm{H_2O} + 2\,\mathrm{CO_2}$$

Simulation was performed for X different cases with varying conditions:

- I. Temperature: 7500K; Pressure in tanks: 10atm,
- II. Temperature: 750K; Pressure in tanks: 15atm,
- III. Temperature: 750K; Pressure in tanks: 20atm,
- IV. Temperature: 750K; Pressure in tanks: 30atm,
- V. Temperature: 1000K; Pressure in tanks: 20atm,
- VI. Temperature: 1000K; Pressure in tanks: 30atm,

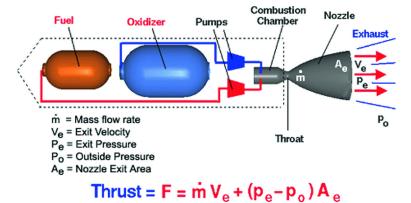


Figure 1: Simplified rocket engine

3 Code overview

Calculation was performed in program created using Python with the implementation of Cantera. At the beginning program defines initial conditions. After that fuel and oxidizer reservoirs are created followed by ignition chamber, nozzle's throat and ignition mechanism. Ignition is cased by free hydrogen radicals. Using

$$A_C H 4 = 4e^- 5m^2$$

- area of the methane injector

$$A_0 2 = 4e^- 5m^2$$

- area of the oxygen injector

$$A_t hroat = 1e^-3m^2$$

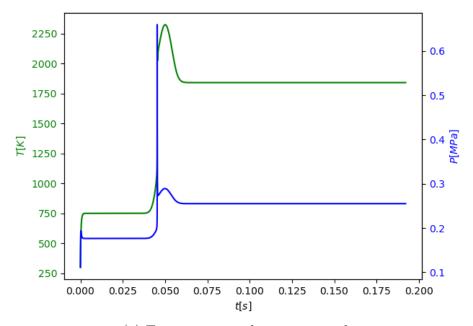
- area of the nozzle's throat program calculates the escape velocity of reaction products

$$v_2 = \sqrt{2T_c \frac{kR}{k-1} \left(1 - \left(\frac{p_2}{p_c}\right)\right)}$$

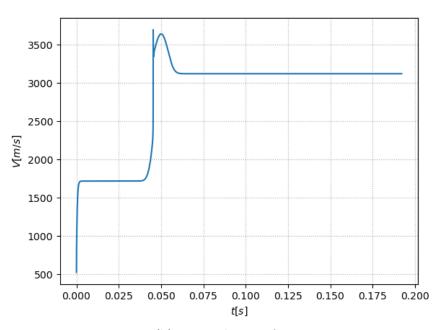
Rest of the parameters, namely temperature, pressure and mass of each of the substrates and products, are calculated by Cantera functions. The results of the calculations are presented on the charts.

4 Results

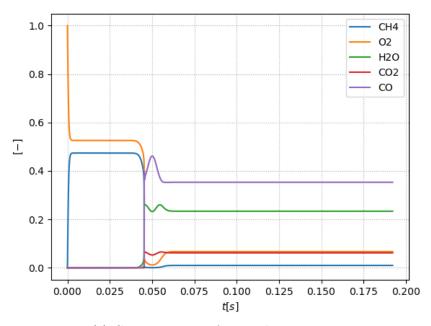
4.1 Case I



(a) Temperature and pressure graph

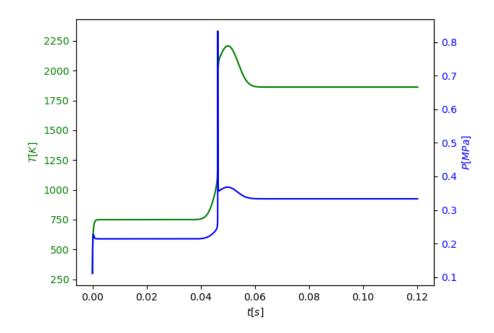


(b) Exit velocity of gases

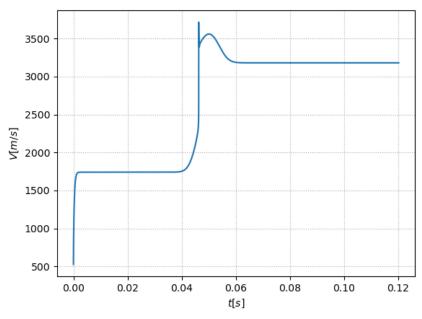


(c) Concentration of gases during reaction Figure 2: Result of Case I

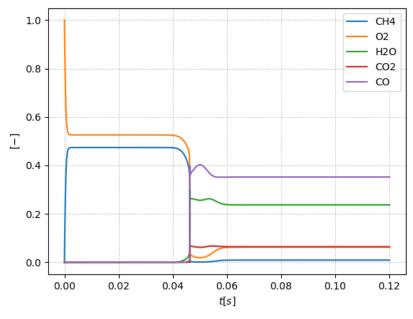
4.2 Case II



(a) Temperature and pressure graph

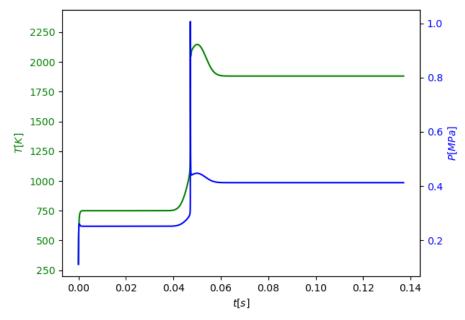


(b) Exit velocity of gases

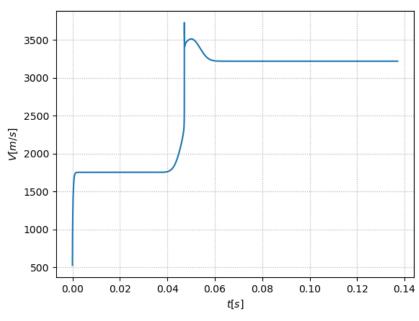


(c) Concentration of gases during reaction Figure 3: Result of Case II

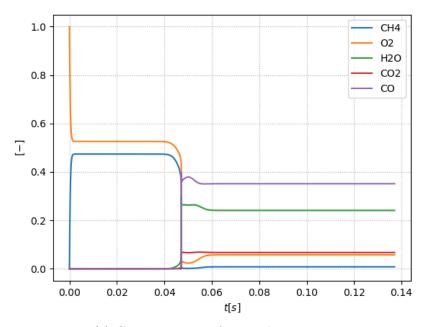
4.3 Case III



(a) Temperature and pressure graph

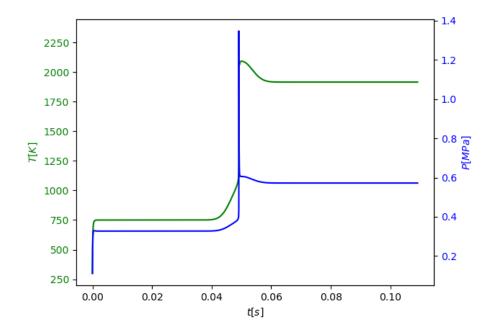


(b) Exit velocity of gases

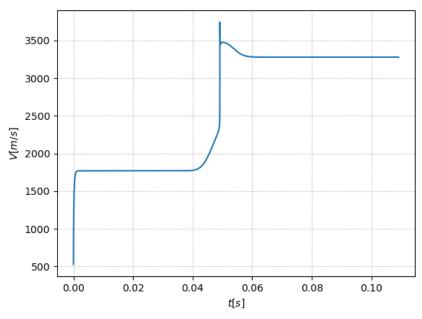


(c) Concentration of gases during reaction Figure 4: Result of Case III

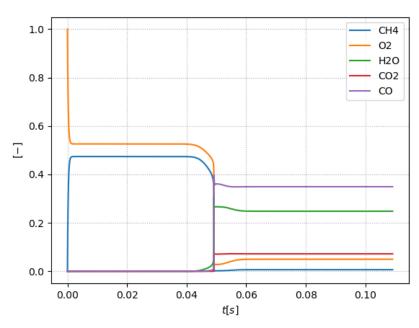
4.4 Case IV



(a) Temperature and pressure graph

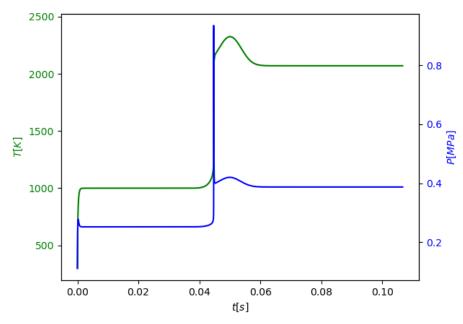


(b) Exit velocity of gases

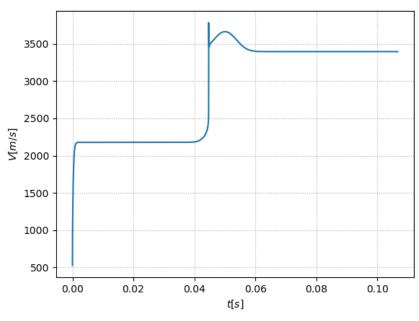


(c) Concentration of gases during reaction Figure 5: Result of Case IV

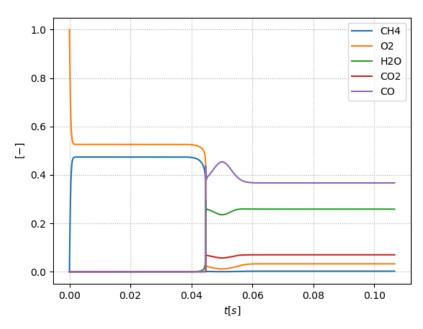
4.5 Case V



(a) Temperature and pressure graph

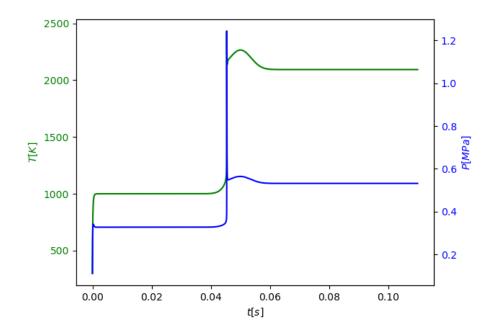


(b) Exit velocity of gases

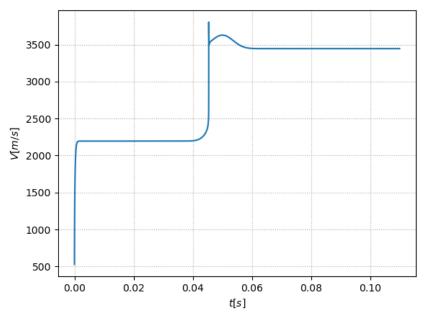


(c) Concentration of gases during reaction Figure 6: Result of Case ${\bf V}$

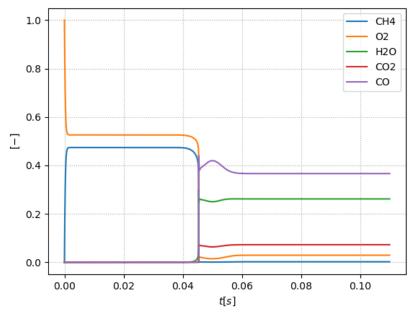
4.6 Case VI



(a) Temperature and pressure graph



(b) Exit velocity of gases



(c) Concentration of gases during reaction Figure 7: Result of Case $\rm VI$

5 Summary

As can be seen after ignition peak of velocity of gases leaving nozzle is achieved. Same things occurs in pressure of the gas. In both cases after the peak, the velocity and pressure stabilize at lower but still much higher than initial value.

As can be expected after ignition concentration of ethane and oxygen lower and concentration of

 H_2O

and CO rises. What is unexpected concentration of

 CO_2

is not very high in comparison to the CO and also some of the oxygen was not used in combustion, which means stechiometric was not achieved.

Maximum temperature is higher for lower initial pressure.

With higher initial pressure there is greater difference in concentration of gases after the ignition.

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