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Combustion of Methan-Oxygen Mixture in Liquid Propellant Rocket Engine

Computer Methods in Combustion

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Contents

1 Introduction

The purpose of the simulation was to investigate combustion of methane in oxygen in liquid propellant rocket. The analysis has been conducted to obtain results of pressure, temperature and gases composition. Additionally the velocity of the exhaust gases is obtained.

The analysis has been implemented in Python using Cantera library with reaction mechanism GRI-Mech 3 which is widely used for homogenous reactions calculations.

2 Model

In the simulation the following assumptions were adopted:

- mass flow rate in the fuel and oxidizer injectors is constant,
- fuel is injected in gas state,
- flow through nozzle is isentropic,
- four reactors are used: fuel, oxidizer, combustion chamber and nozzle
- all reactors are 0-dimensional.

The boundary conditions are as follows:

- fuel - methane ($T = 293K$, $p = 40atm$),
- oxidizer - oxygen ($T = 293K$, $p = 40atm$),
- combustion chamber virtual volume - $V = 5 \cdot 10^{-4} m^3$,
- ignition is caused by injection of free hydrogen radicals which flow rate decrease exponentially.

Area of outlet of the fuel injector, area of outlet of oxidizer injector and area of throat of the nozzle are as follows:

- area of fuel injector $A_{fuel} = 4 \cdot 10^{-5} m^2$
- area of oxygen injector $A_{O_2} = 4 \cdot 10^{-5} m^2$
- area of throat of the nozzle $A_{throat} = 1 \cdot 10^{-5} m^2$

The stechiometric equation for methane and oxygen combustion is as follows:

$$CH_4 + 2O_2 = CO_2 + 2H_2O \tag{1}$$

The molar ratio is 2:1, thus the mass ratio is 4:1.
In this calculations mass ratio is 1,41 so the mixture is very rich.

Figure 1: simplified rocket engine diagram

3 Program structure

In the beginning the program creates reactants and define their pressure, temperature and chemical composition. Next the valve coefficient is computed. It is needed for setting pressure difference between reservoirs. The function which calculate this is based on critical flow in the nozzle. In consequence the mass flow between reservoirs depends only on area of throat and specific gas constant and its value is constant.

The velocity of exhaust gases in each iteration are calculated from:

$$v_2 = \sqrt{2 \cdot \frac{kR}{k-1} \cdot T_0 \cdot \left[1 - \left(\frac{p_2}{p_0}\right)^{\frac{k-1}{k}}\right]} \tag{2}$$

4 Results

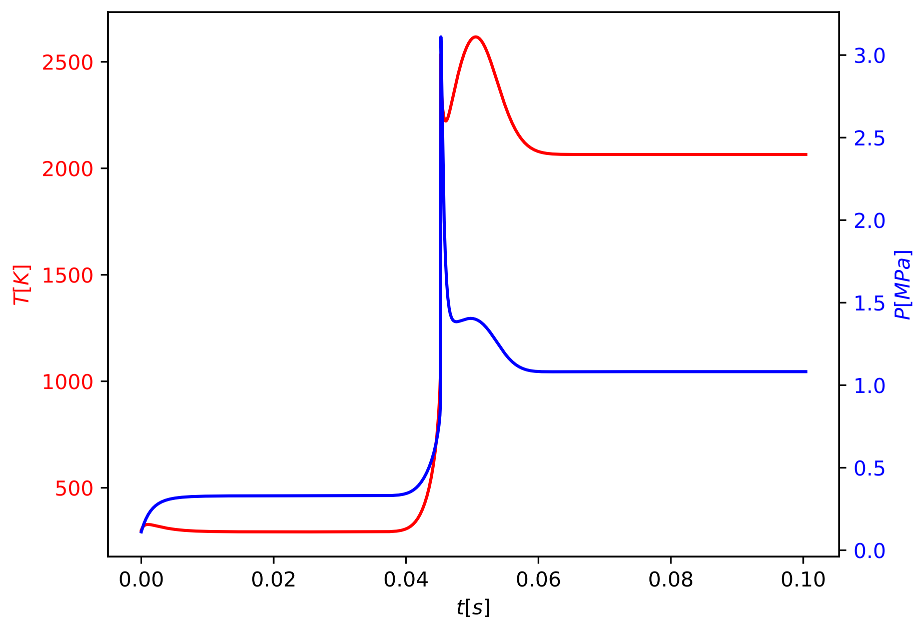

Figure 2: temperature & pressure

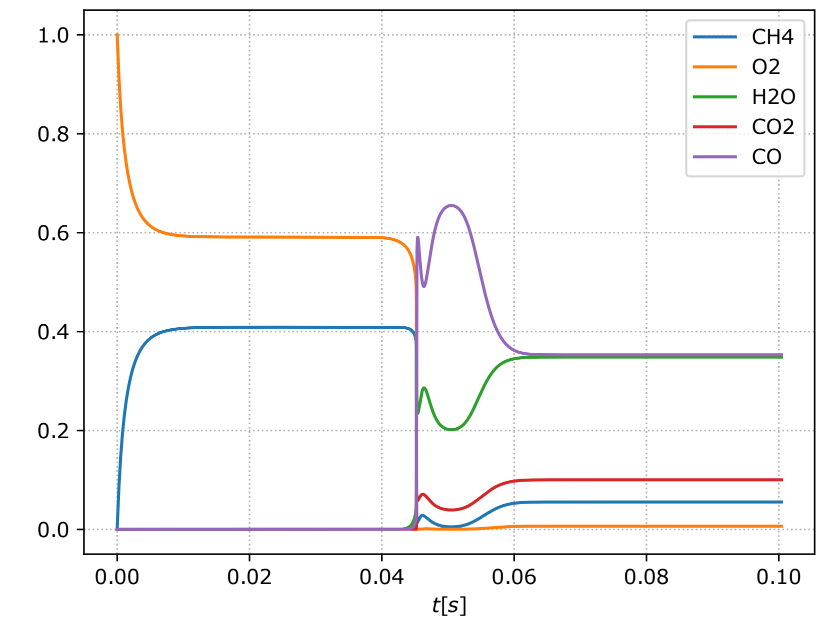

Figure 3: composition of reagents in combustion chamber

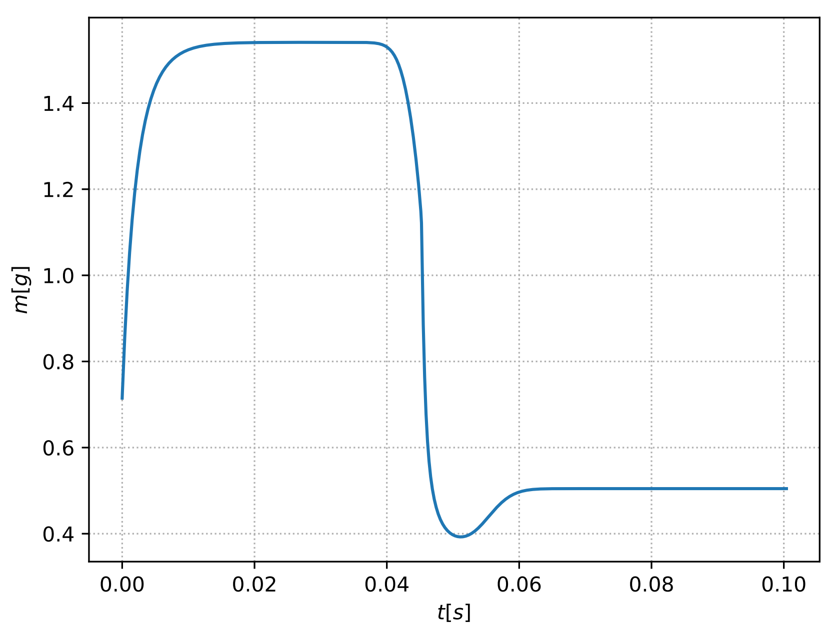

Figure 4: mass of reagents in combustion chamber

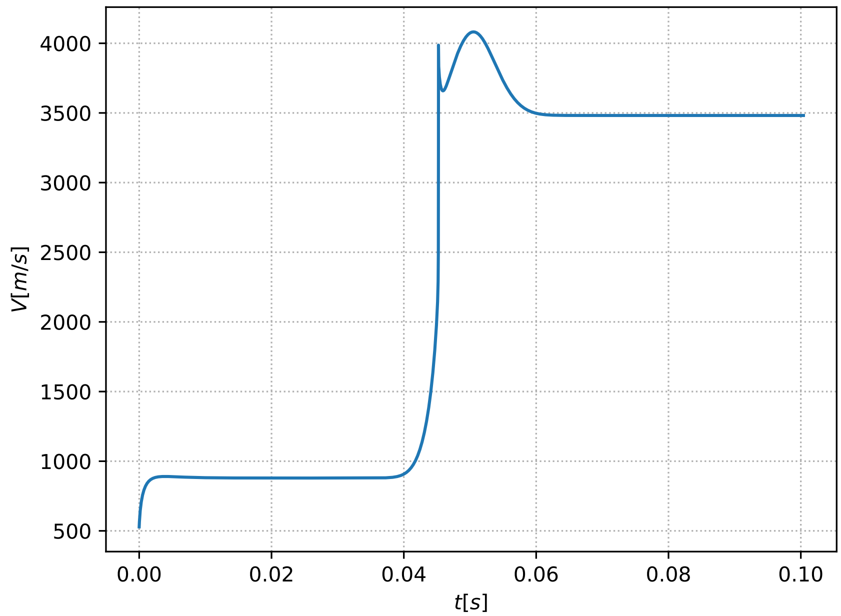

Figure 5: velocity

5 Summary

The gases in combustion chamber contain large amount of CO and low amount of O_2. The mixture is very rich, so it was predictable that combustion is incomplete.

The peak of temperature and pressure is caused by injection of hydrogen radicals into the chamber which started an ignition.

It is also noticeable, that as the ignition began, mass of reagents started to decrease rapidly.

This analysis is simplified, but it can be a good foundation for further calculations and experiments.

6 Sources

1. https://github.com/mranachowski/cantera_rocket_engine

2. https://cantera.org/documentation/dev/sphinx/html/cython/zerodim.html