Politechnika Warszawska

Wydział Mechaniczny Energetyki i Lotnictwa

Metody Komputerowe w Spalaniu

Symulation of combusting a fuel and air mixture in variable volume with spontaneous ignition

Author:
Mateusz Skrobek

Supervisor:
Dr. Mateusz Żbikowski

April 25, 2018

1 Introduction

Examination of spontaneous ignition is extremely important in order to avoid unexpected ignitions or explosions dangerous, explosive materials. In my studies I focused on three types of inflammable compounds – mixtures of air and methane, ethane and propane. The purpose of my examination was to scrutinize fuel's reaction to different temperatures of walls of the reactor with movable piston and to designate boundary temperature of spontaneous ignition for all these compounds.

2 Model description

2.1 Software

Software used for conducting the study was an open-source chemical kinetics software – Cantera. It is written in C++ and can be used from C++, Python, Matlab and Fortran. I used Python.

2.2 Variable volume reactor model

To illustrate actual model of reactor I created two gas 'Reactors', first (combustor) with fuel - mixture of air and methane/ethane/propane – and second with air. Between them I put movable 'Wall' which symbolize the piston.
Initial thermodynamic properties and volume in both reactors are the same – 27°C(300,15K), one atmosphere pressure and 0,5 m^3 each.
I made my program customizable – every user at the beginning is asked to enter the type of fuel, new value of temperature of the combustor's walls and time interval between measurements.

2.3 Order of activities

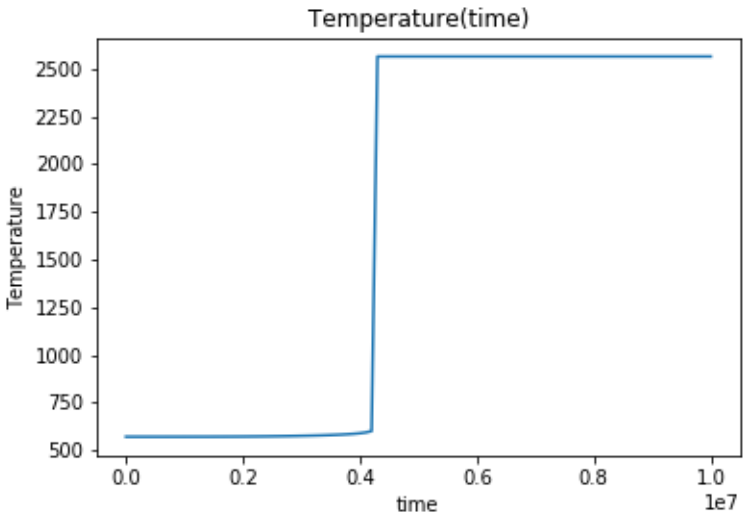
After receiving values from user program has all necessary data and is able to create simulation ('ReactorNetwork') with two reactors. Afterwards program calculates physical quantities (temperature, pressure and volume) of the combustor in time (101 steps with time interval entered by user before) and prints them. Next, thanks to MatPlotLib (Python library), program draws 2D plots of physical quantities depending on time. At the end I put condition which tells the user if auto-ignition has occurred.

3 Results

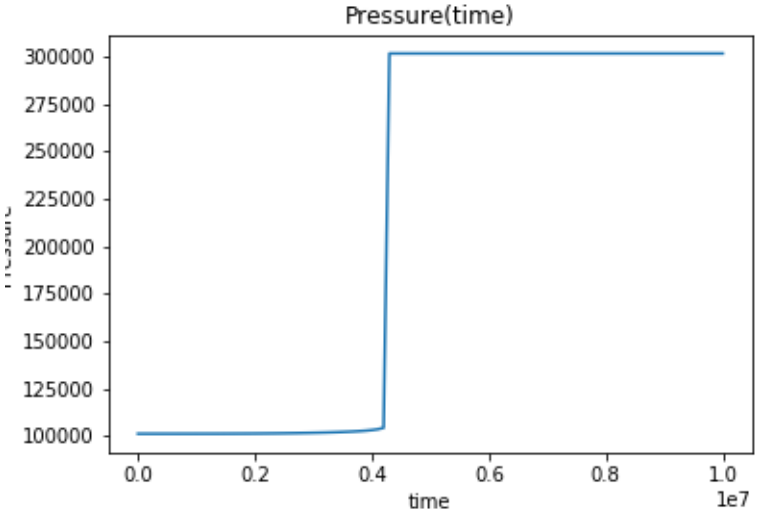
I was examining spontaneous ignition for every hydrocarbon by trial and error – checking different temperatures and validate outcome. I made 6 measurements for each fuel.
As a benchmark I used the spontaneous ignition temperature form Material Safety Data Sheet (MSDS) to compare my results and real values. The final results were quite surprising – auto-ignition has occurred even in relatively low temperatures, but time required to reach auto-ignition and temperature leap was extremely long – spontaneous ignition took place after about 10^6 – 10^7 seconds.
Below I present my plots and table with measured combustion temperature depending on initial temperature of reactor's walls.

3.1 CH_4

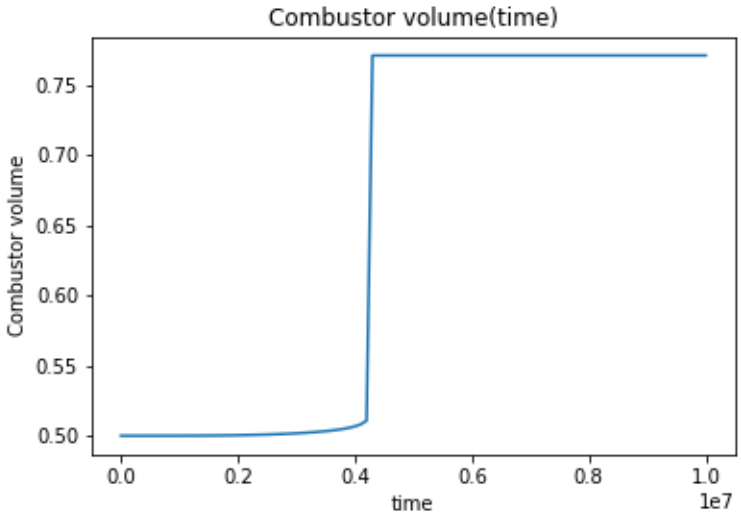
3.1.1 570K



Temperature plot

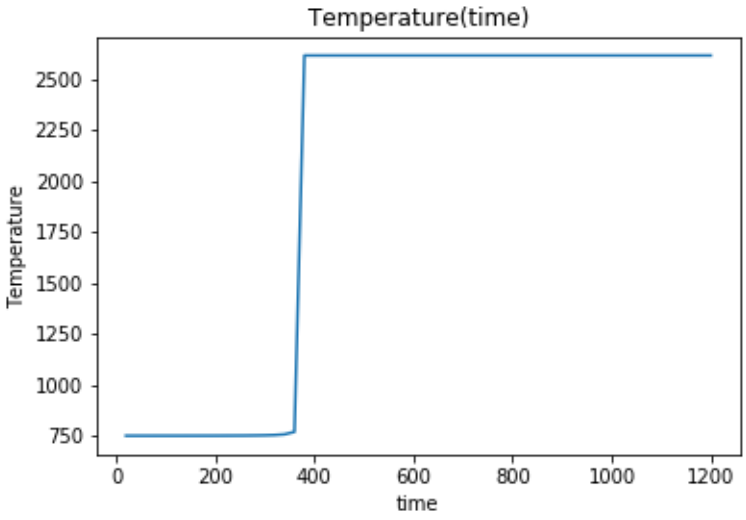


Pressure plot

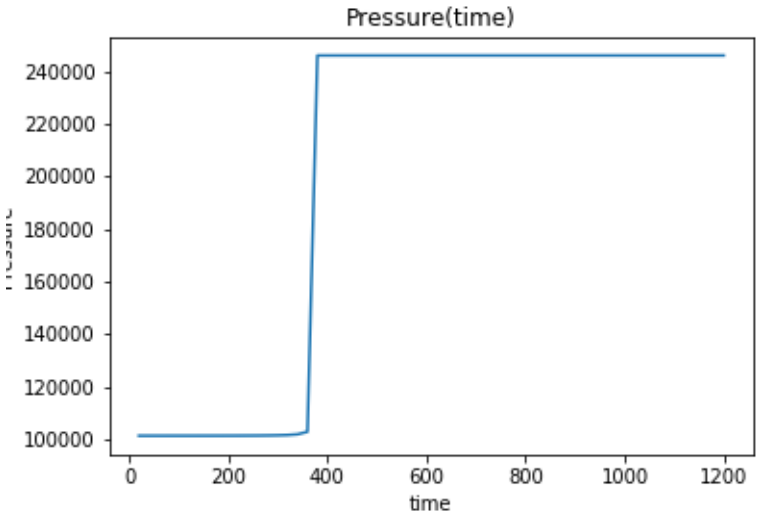


Volume plot

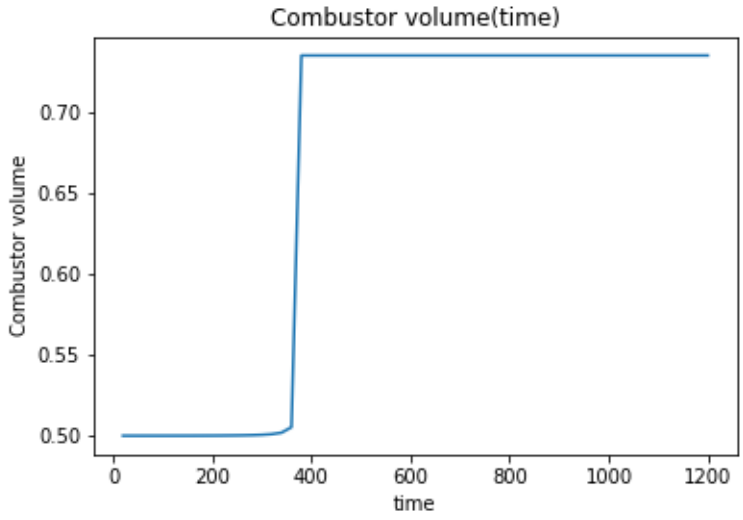
3.1.2 750K



Temperature plot

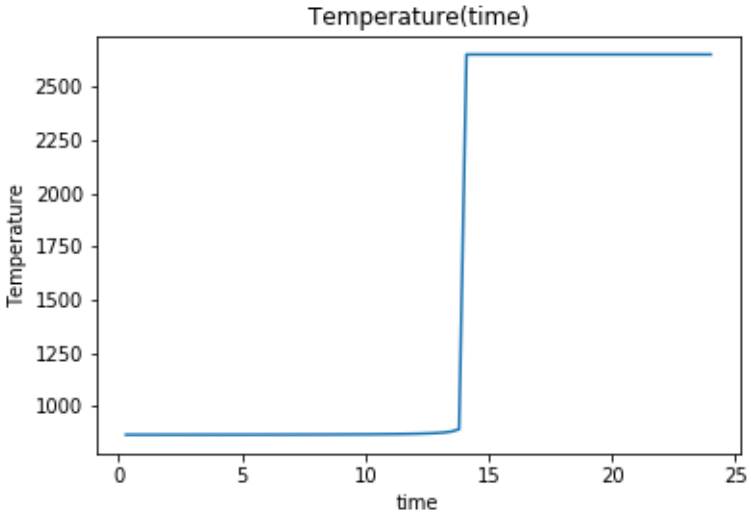


Pressure plot

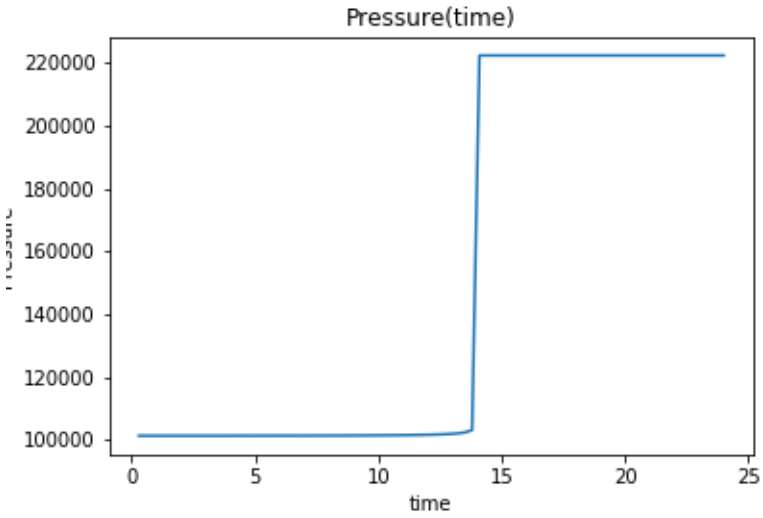


Volume plot

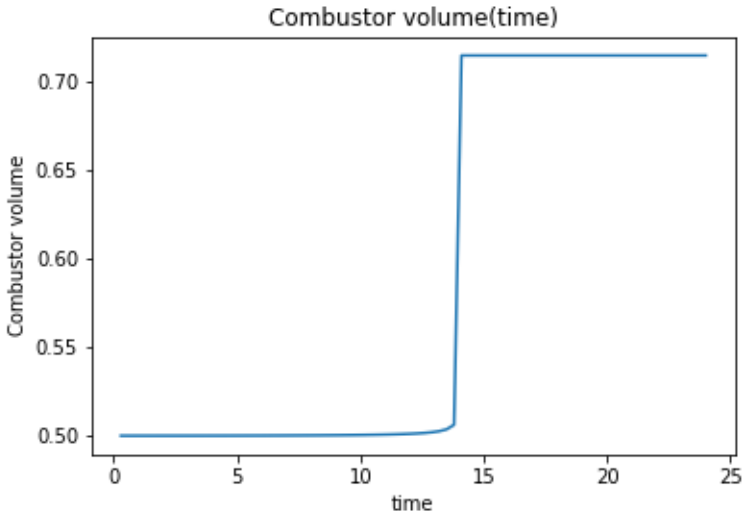
3.1.3 868K



Temperature plot

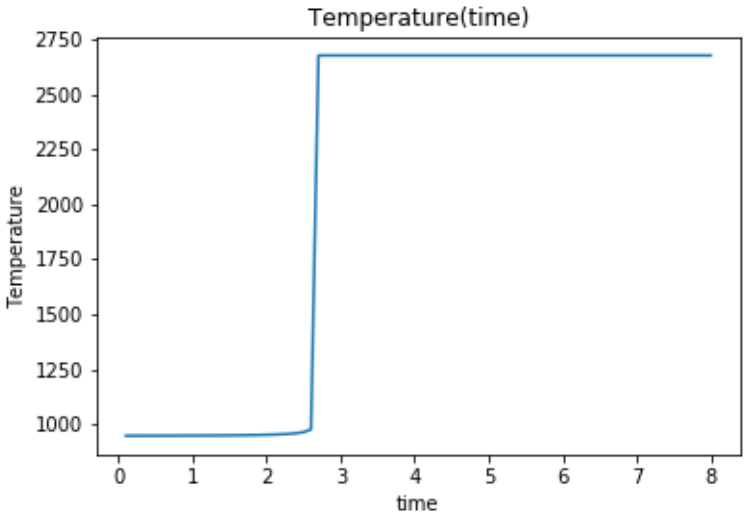


Pressure plot

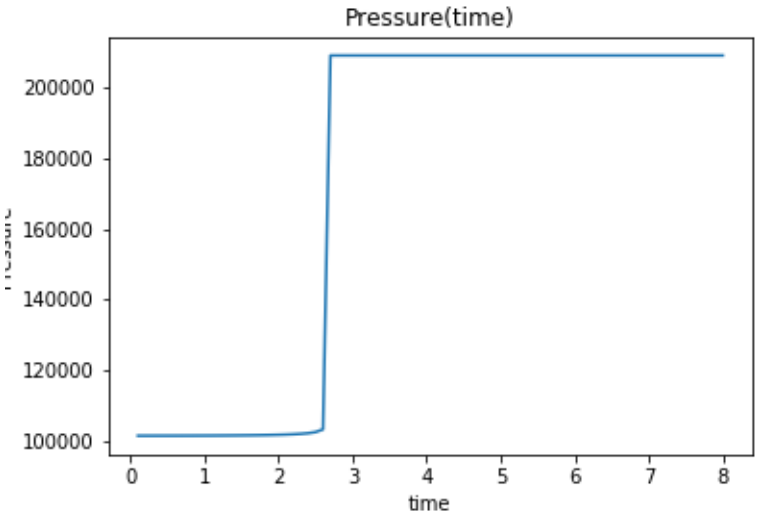


Volume plot

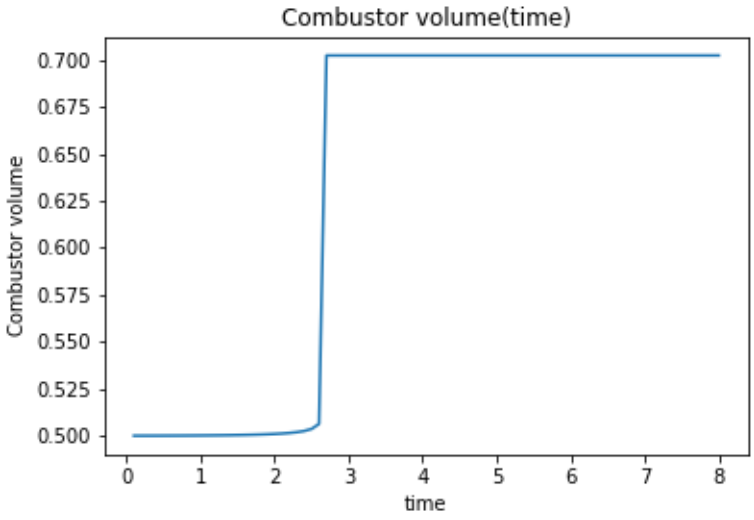
3.1.4 950K



Temperature plot

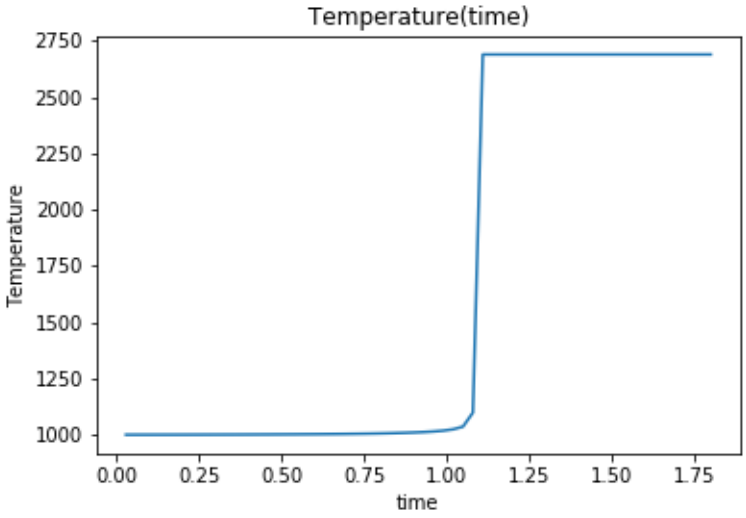


Pressure plot

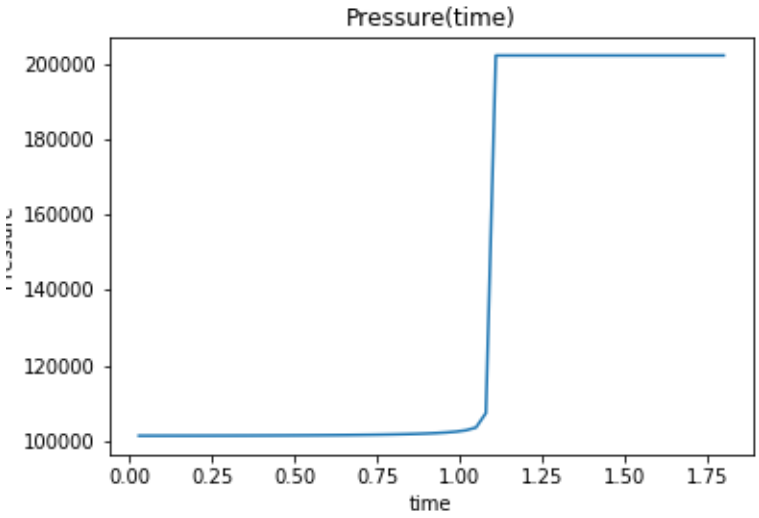


Volume plot

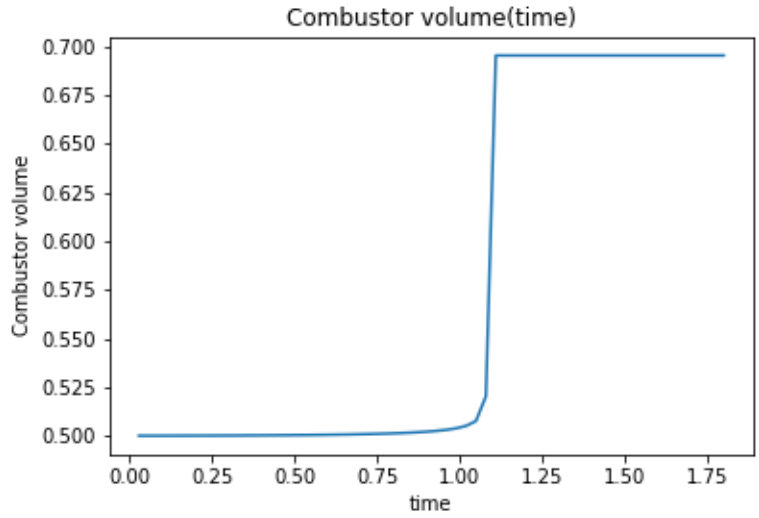
3.1.5 1000K



Temperature plot

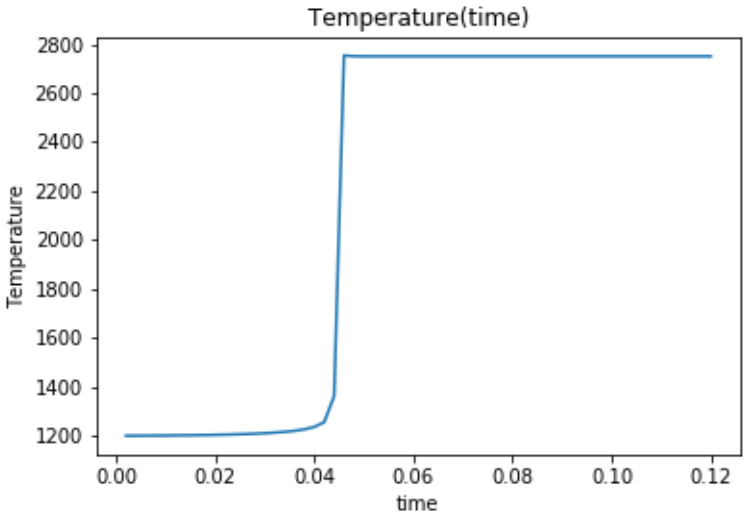


Pressure plot

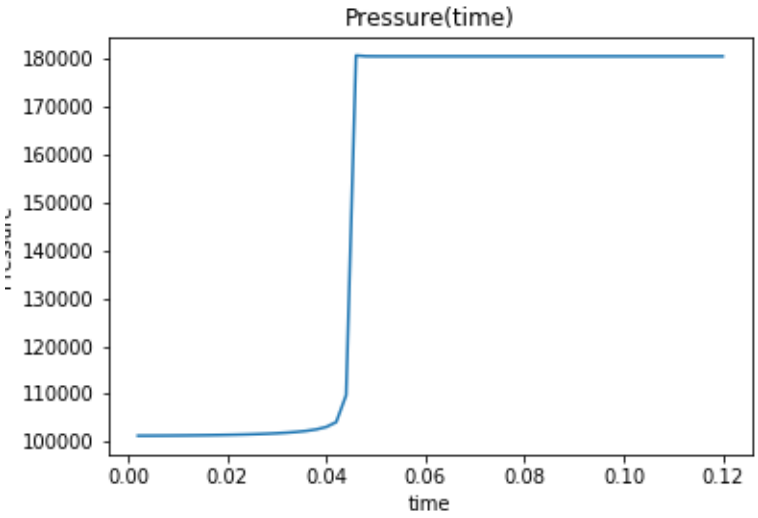


Volume plot

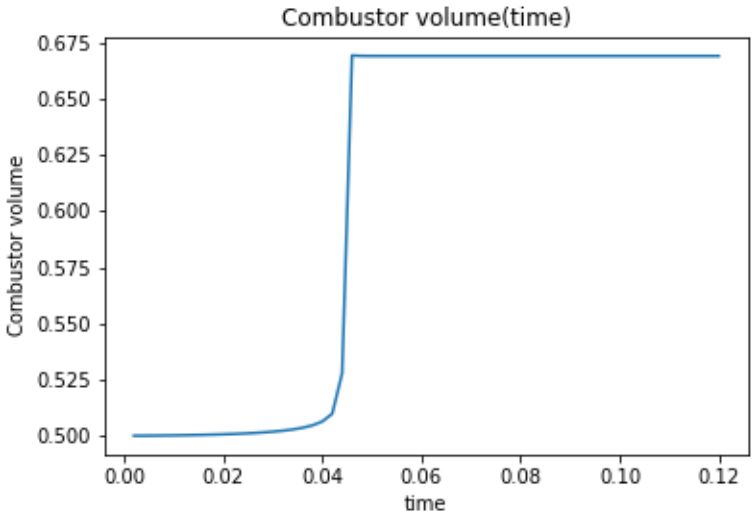
3.1.6 1200K



Temperature plot



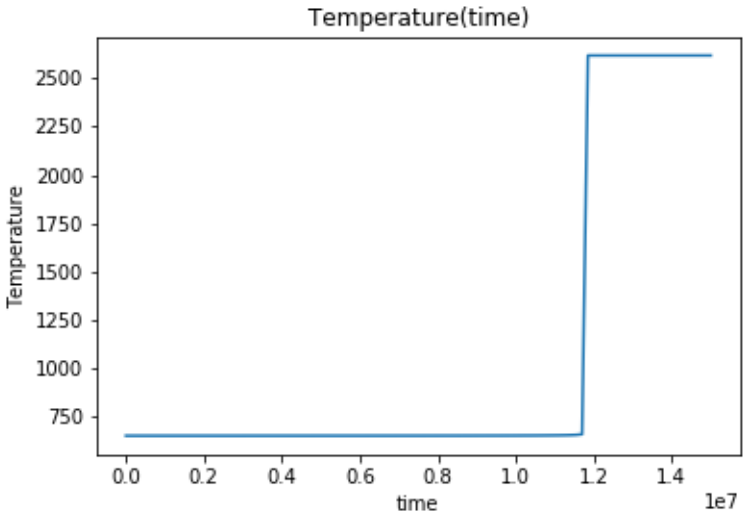
Pressure plot



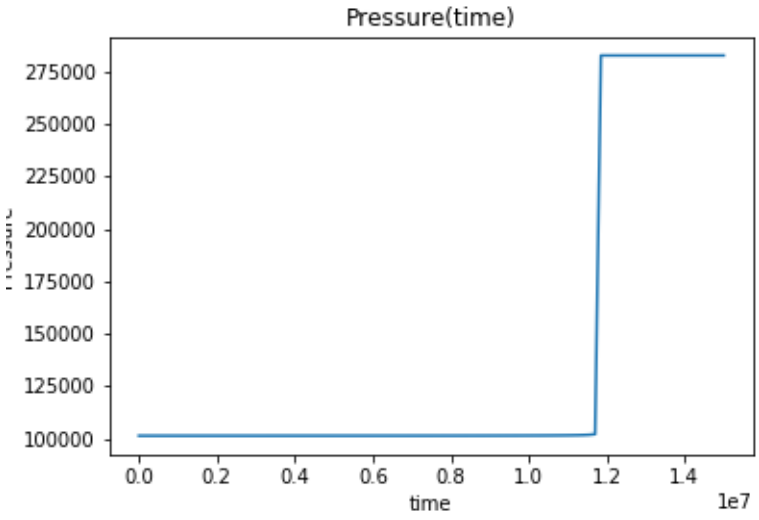
Volume plot

3.2 C_2H_6

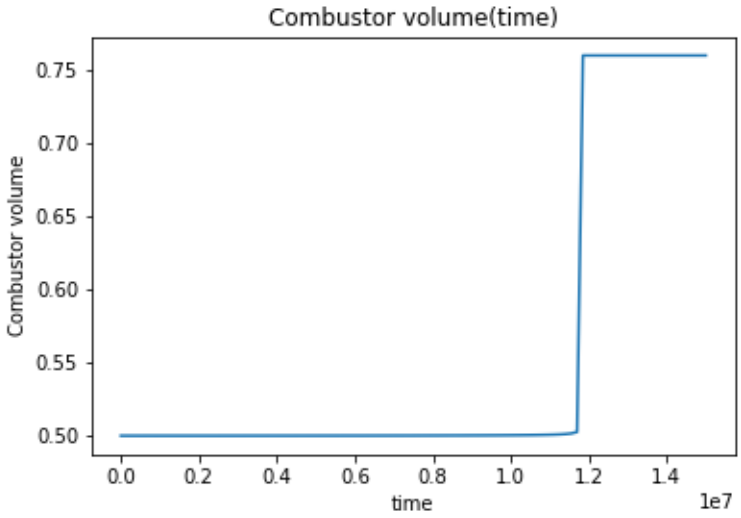
3.2.1 650K



Temperature plot

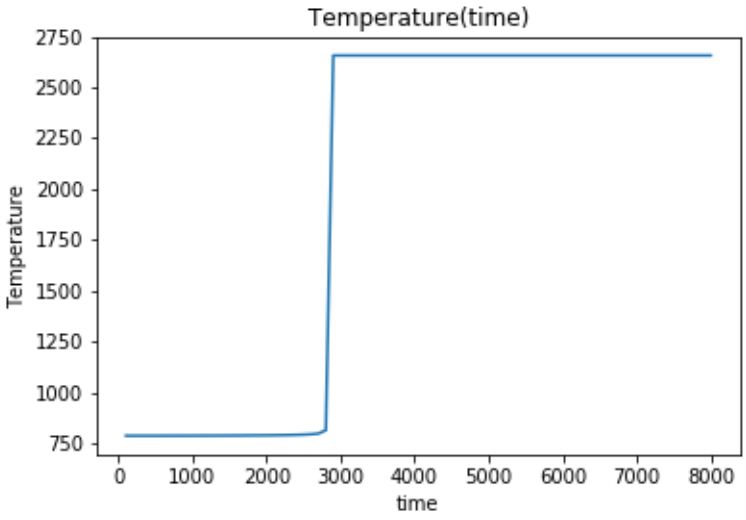


Pressure plot

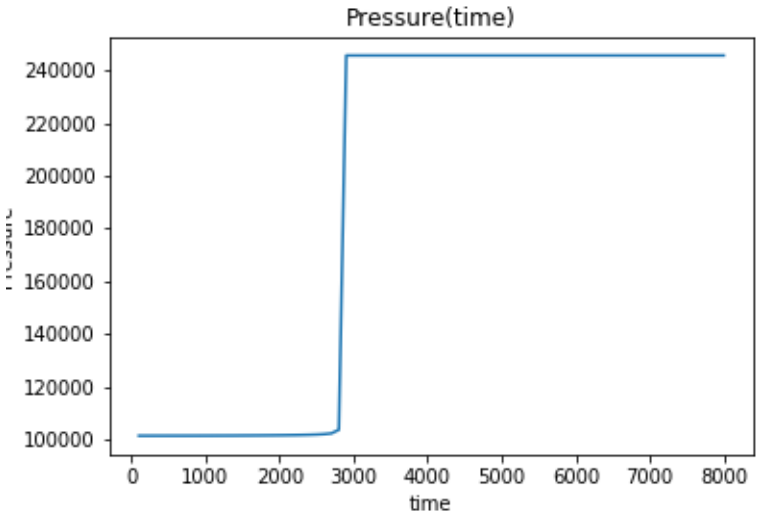


Volume plot

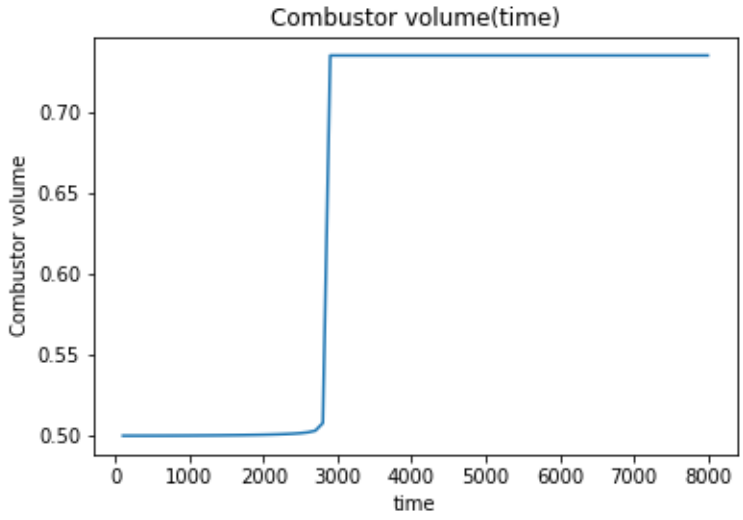
3.2.2 788K



Temperature plot

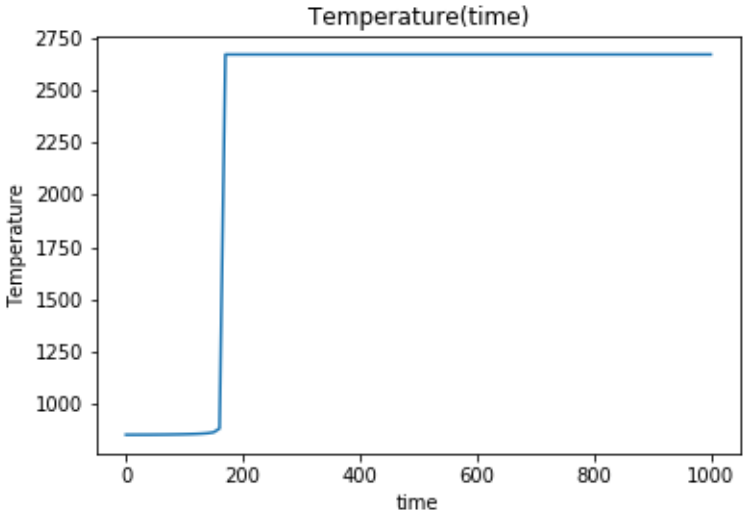


Pressure plot

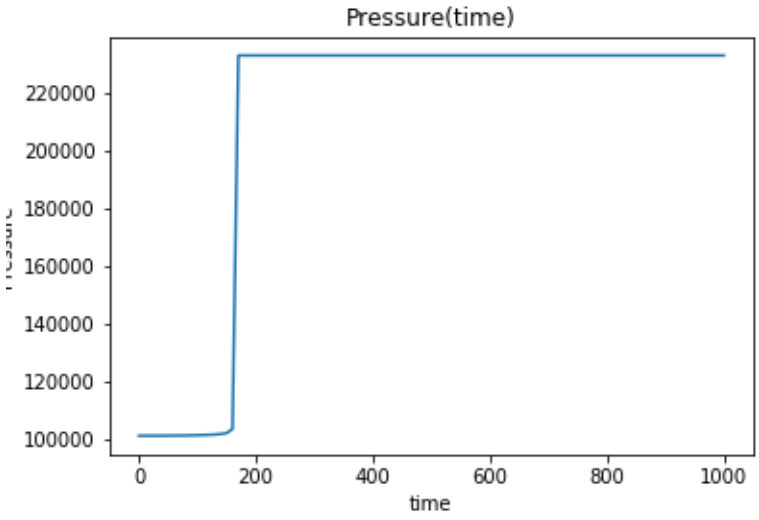


Volume plot

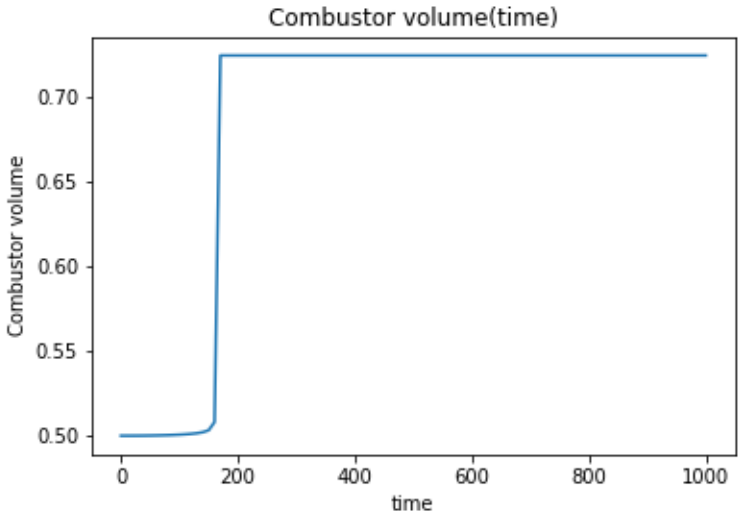
3.2.3 850K



Temperature plot

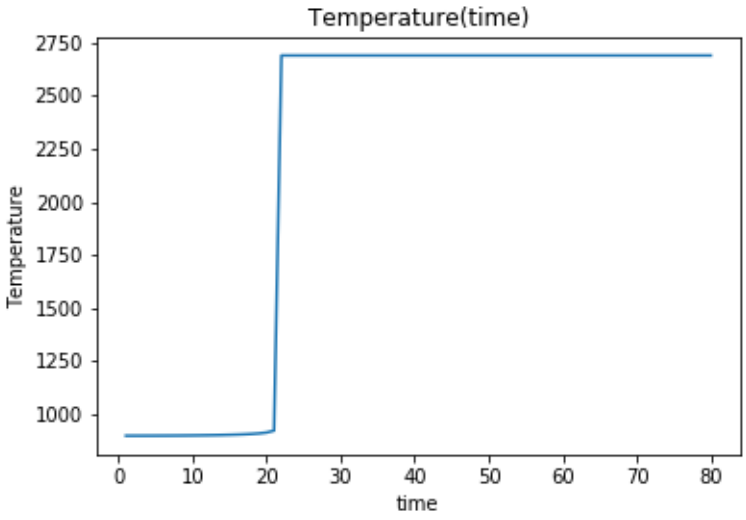


Pressure plot

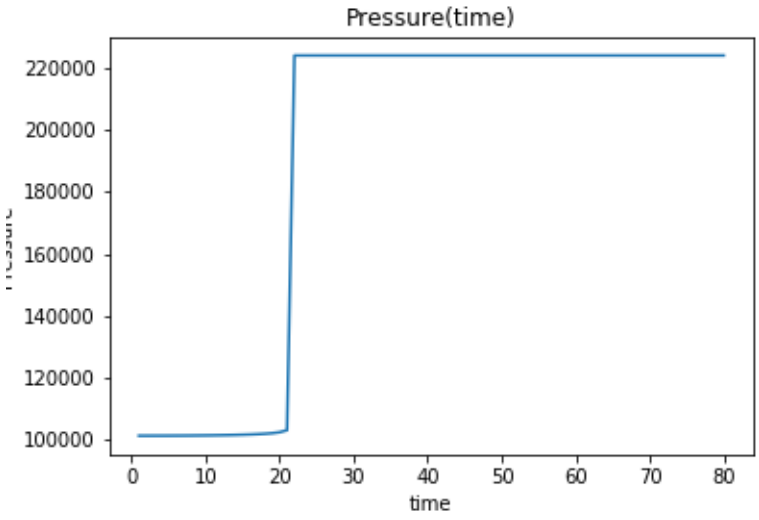


Volume plot

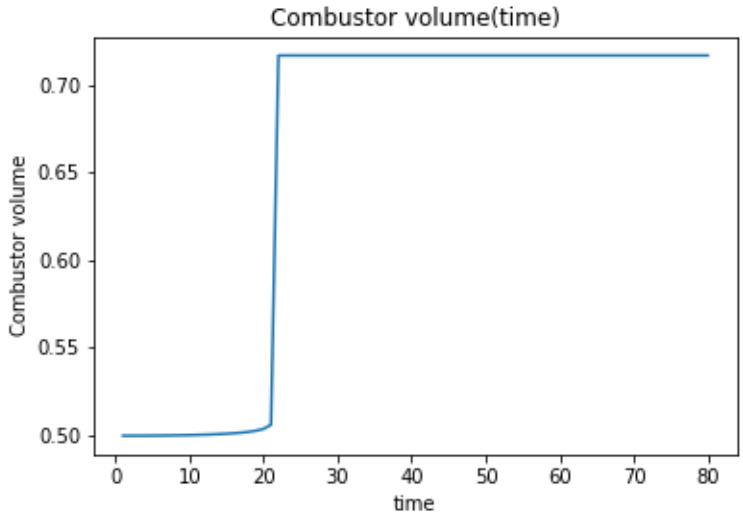
3.2.4 900K



Temperature plot

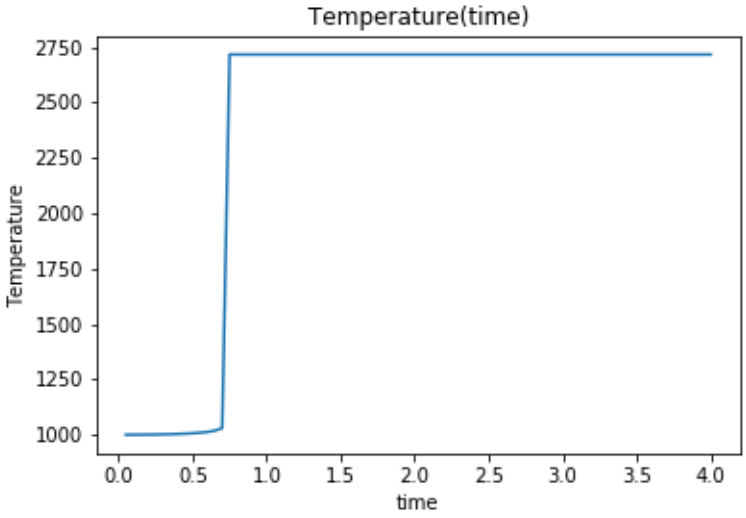


Pressure plot

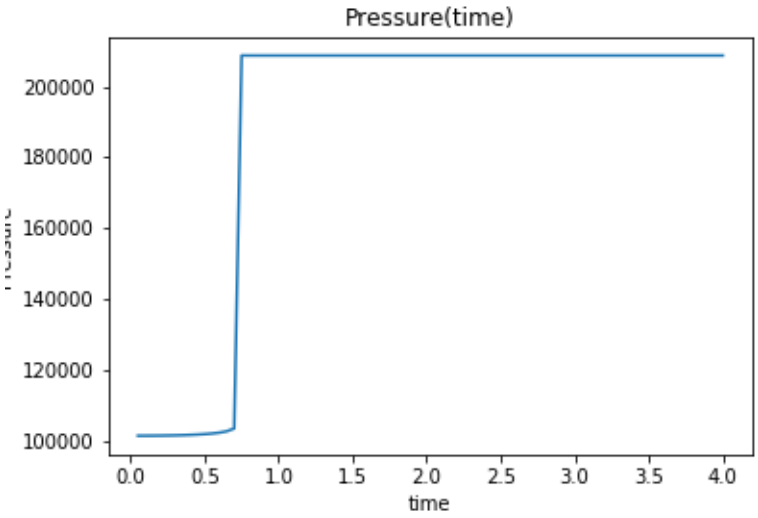


Volume plot

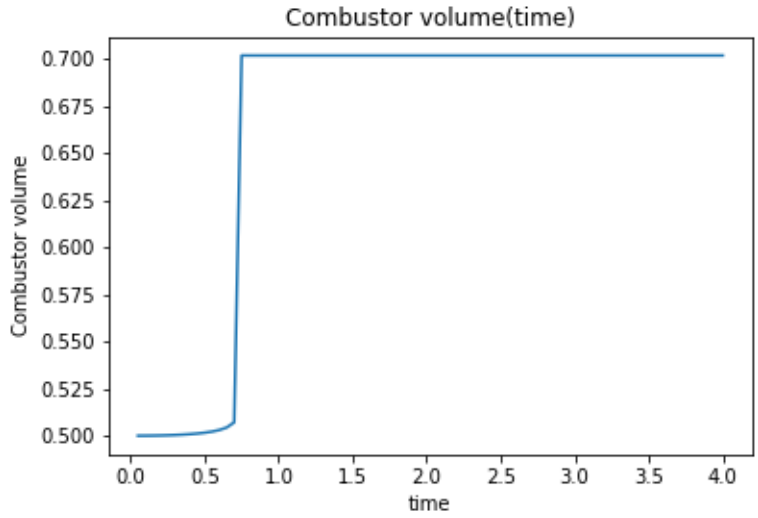
3.2.5 1000K



Temperature plot

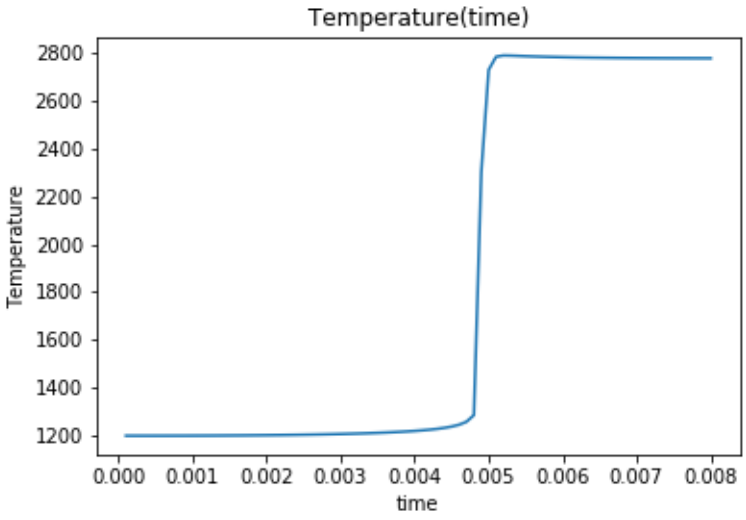


Pressure plot

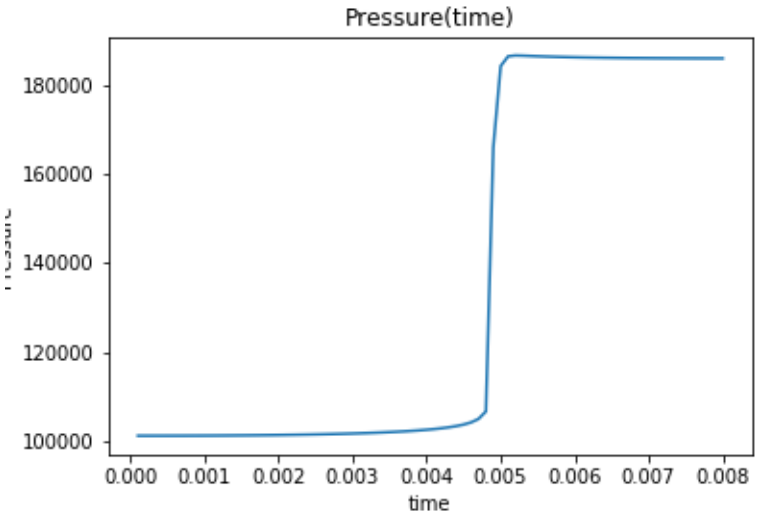


Volume plot

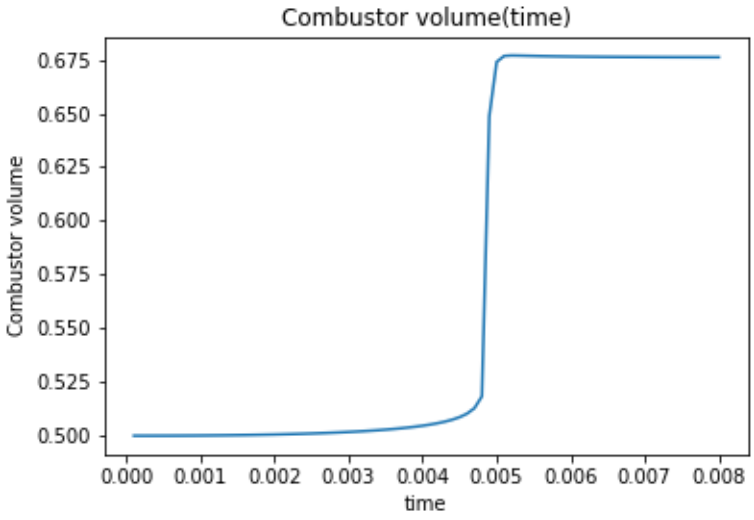
3.2.6 1200K



Temperature plot



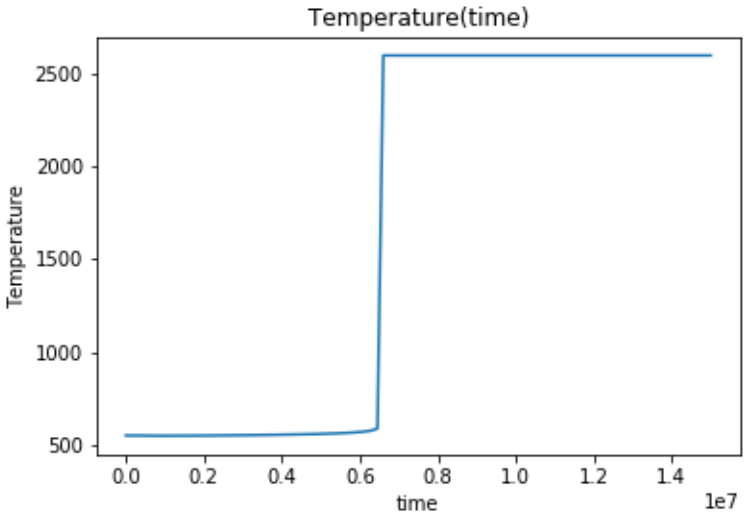
Pressure plot



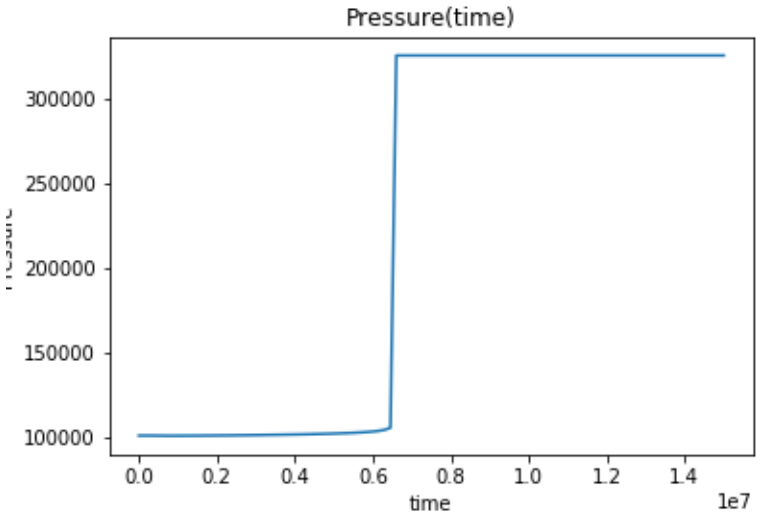
Volume plot

3.3 C_3H_8

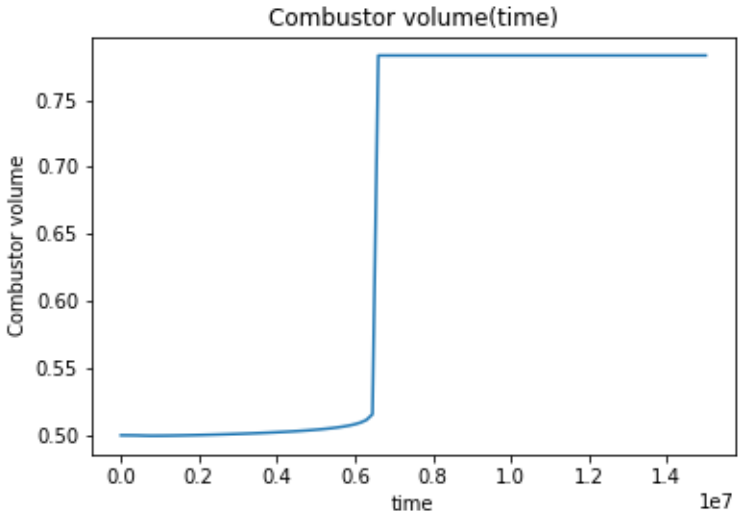
3.3.1 550K



Temperature plot

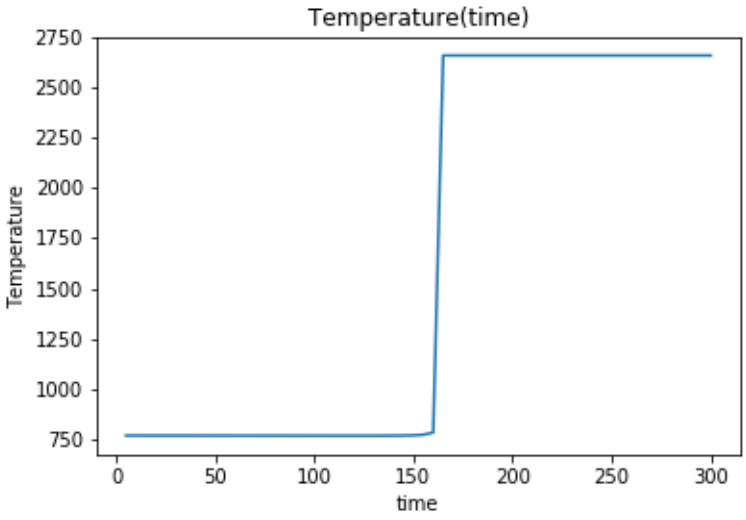


Pressure plot

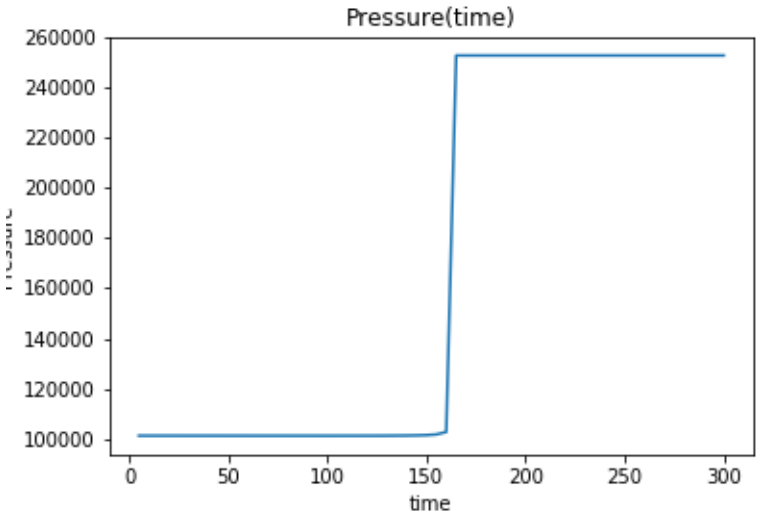


Volume plot

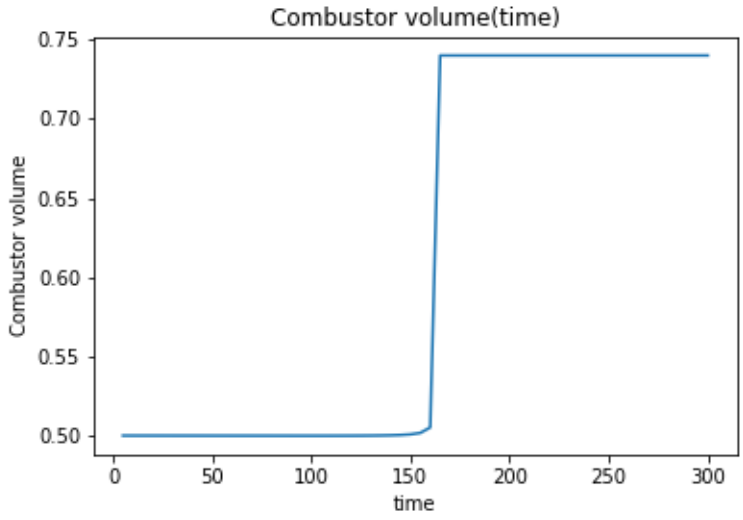
3.3.2 743K



Temperature plot

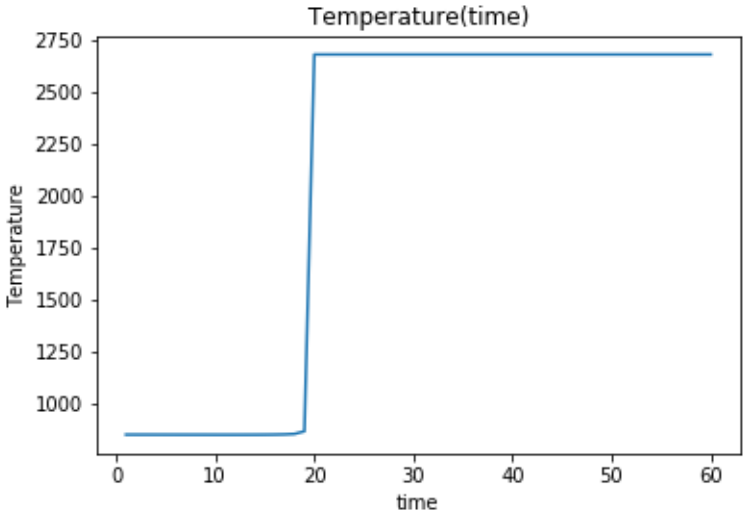


Pressure plot

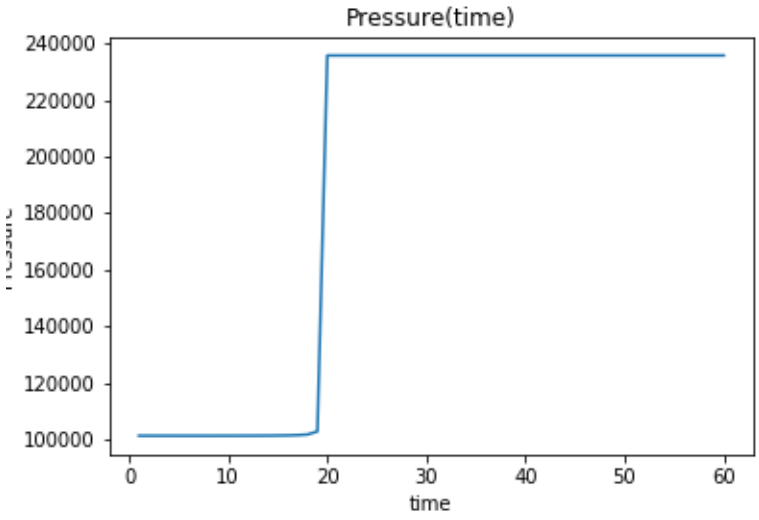


Volume plot

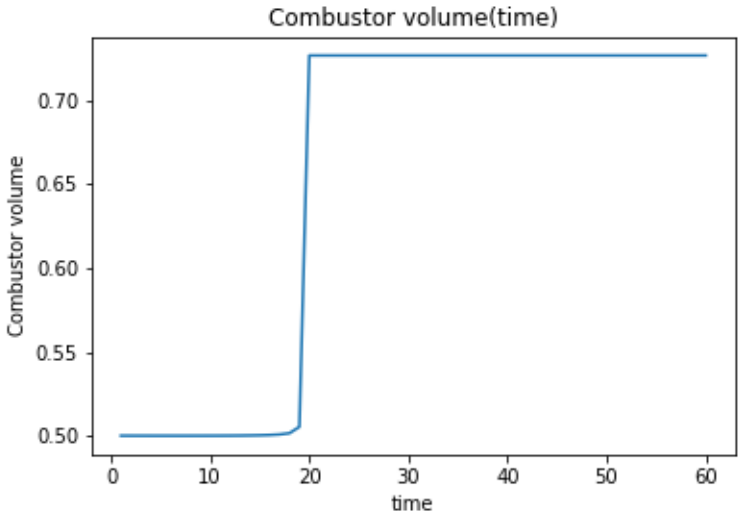
3.3.3 850K



Temperature plot

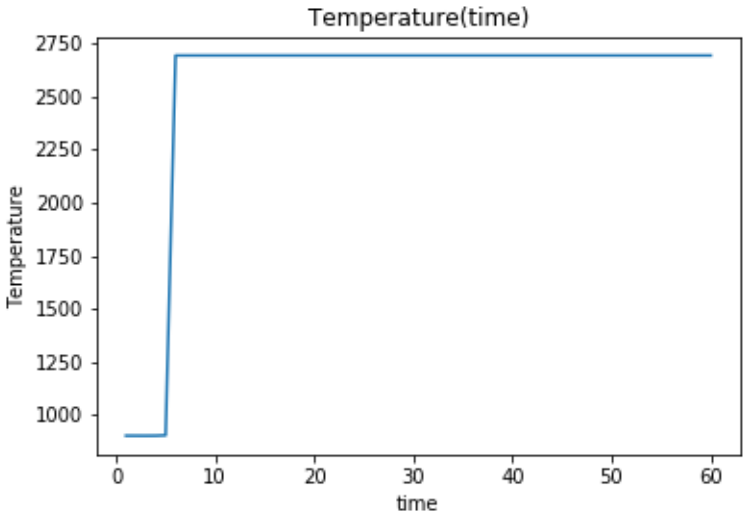


Pressure plot

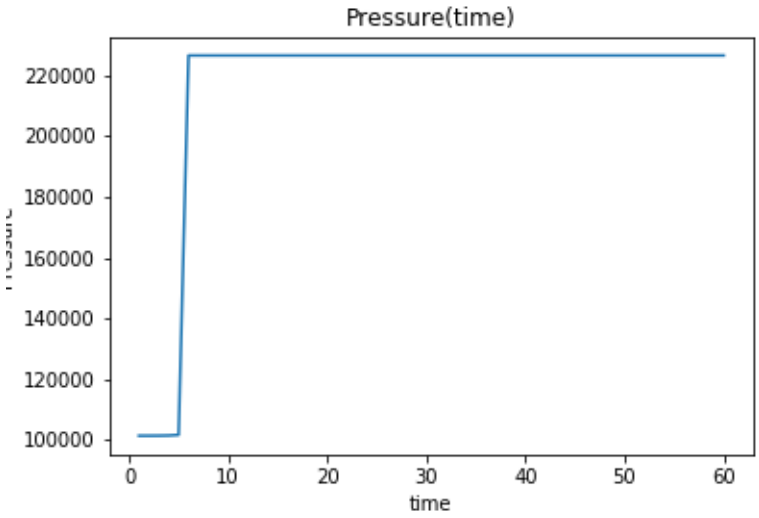


Volume plot

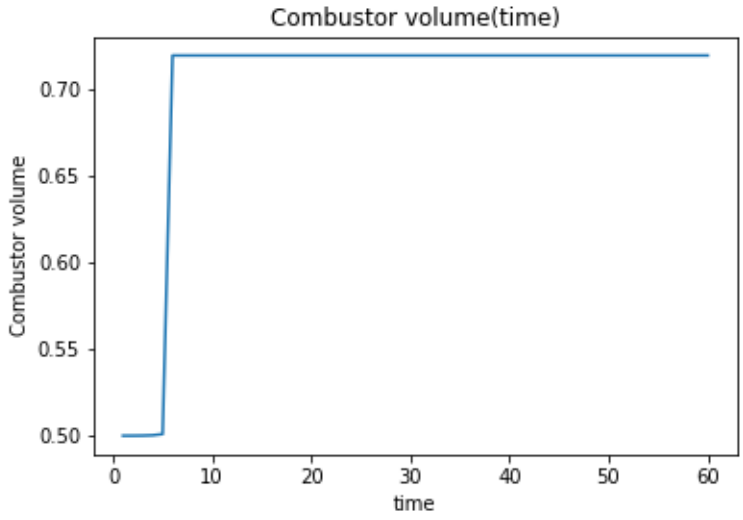
3.3.4 900K



Temperature plot

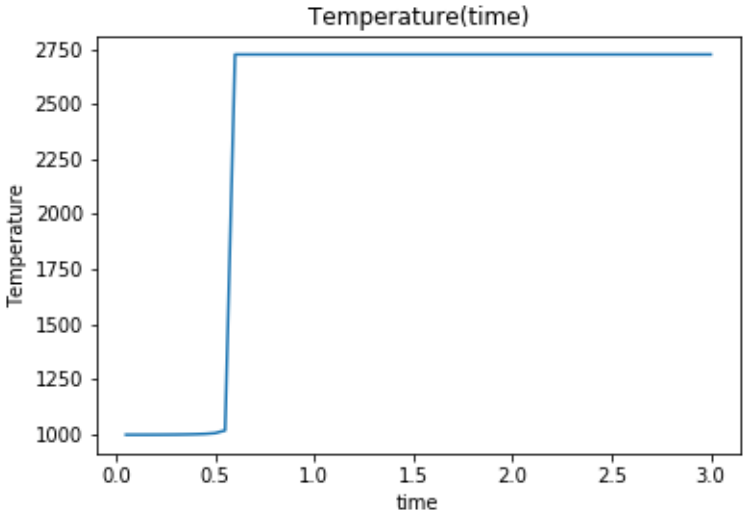


Pressure plot

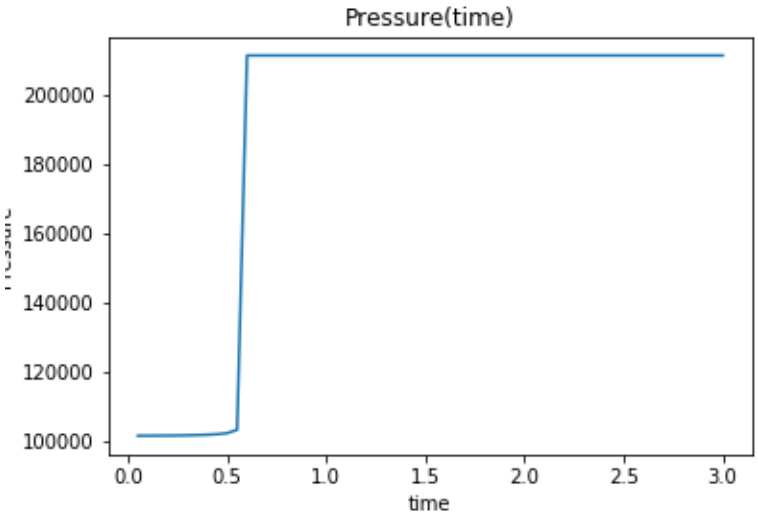


Volume plot

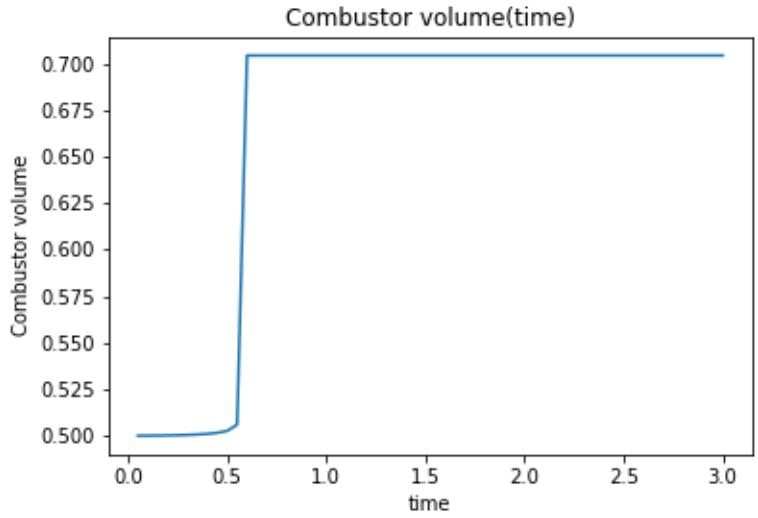
3.3.5 1000K



Temperature plot

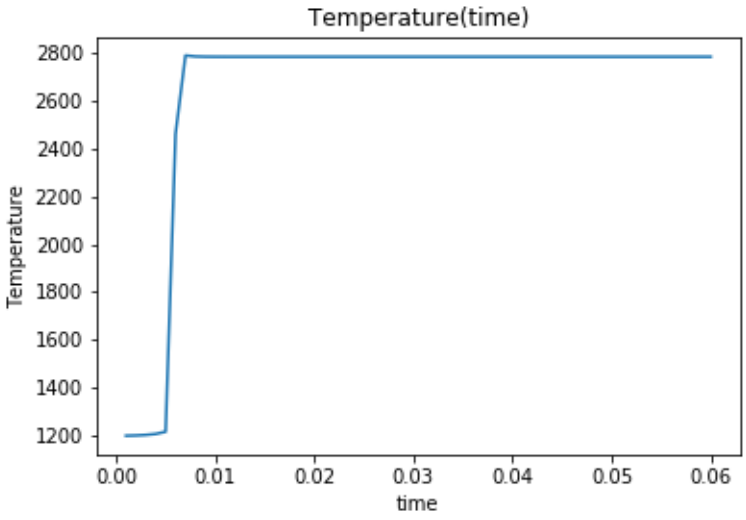


Pressure plot

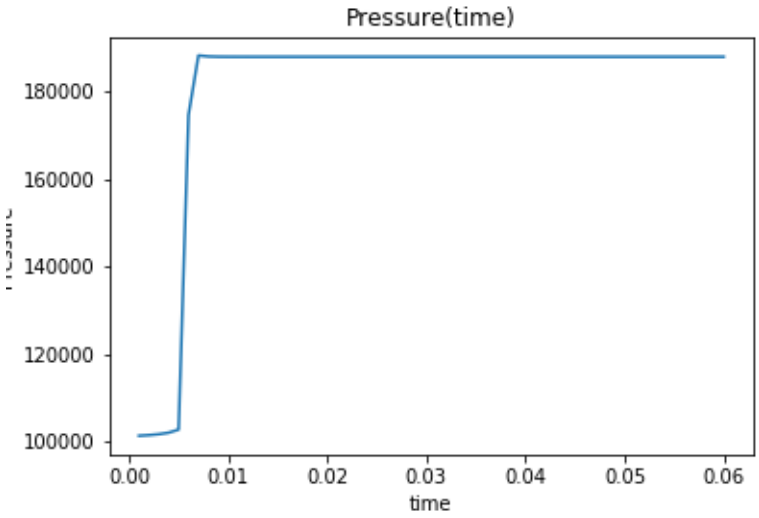


Volume plot

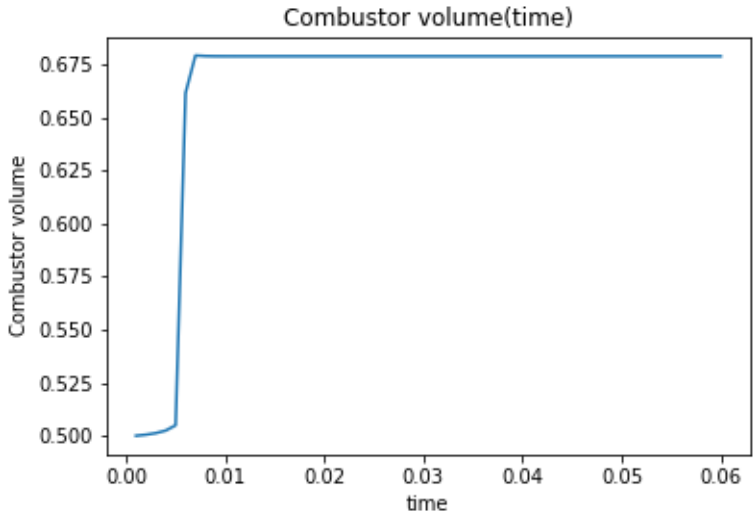
3.3.6 1200K



Temperature plot



Pressure plot



Volume plot

Combustion temperature					
CH4		C2H6		C3H8	
570K	2565K	650K	2590K	550K	2602K
750K	2615K	788K	2656K	743K	2658K
868K	2642K	850K	2673K	850K	2680K
950K	2675K	900K	2688K	900K	2695K
1000K	2690K	1000K	2717K	1000K	2724K
1200K	2750K	1200K	2776K	1200K	2776K

4 Analysis and summary

Accoridng to data from MSDS from 'Linde Gas Polska' auto-ignition temperatures for hydrocarbons are: 868K for CH_4, 788K for C_2H_6 and 743K for C_3H_8.
If we compare it with my calculations it is easy to deduce that there are some discrepancies. In every case calculated temperature is lower than estimated one. Important fact is that in low temperatures the time needed to spontaneous ignition is extremely big and in temperatures from MSDS it is tens or hundreds of seconds.

My calculations may be inaccurate due to limited random-access memory. Also it is unclear how to interpret temperature of spontaneous ignition. Is it limited by time?
Because of enormous periods of time in low temperatures I can assume and conclude that useful results when auto-ignition occurs after tens of seconds, so cross-border temperatures for my hydrocarbons are: ca. 800K for CH_4, ca. 900K for and ca. 850K for C_3H_8, so it is approximately similar to actual values.
Another conclusion is quite simple. Making use of the table I can say that the higher initial temperature the higher combustion temperature is, but inequalities are not big. I can say it is 2650K +/- 100K for every hydrocarbon.

5 Bibliography

cantera.org/docs/sphinx/html/cython/index.html
cerfacs.fr/cantera/docs/cantera/dgoodwin_reactors.pdf
linde.pl/pl/index.html
stackoverflow.com/