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

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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.

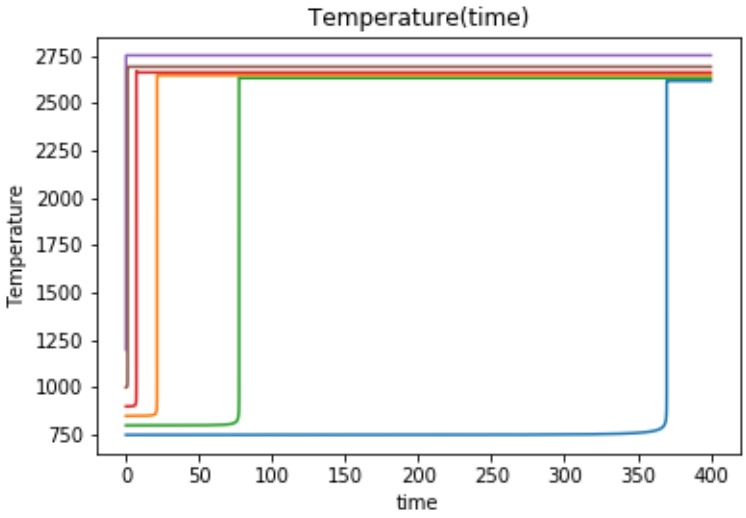
2.3 Order of activities

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.

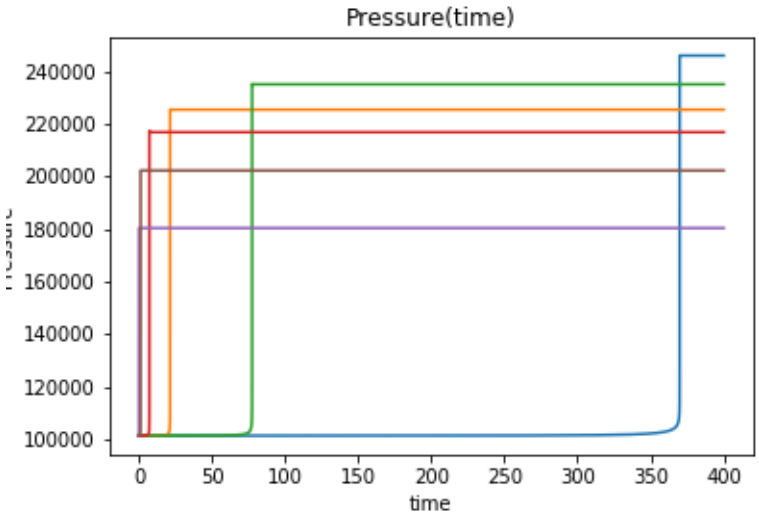
3 Results

I examined spontaneous ignition for every hydrocarbon by checking different temperatures and validating outcome. I made six measurements for each fuel - six temperatures were considered: 750K, 800K, 850K, 900K, 1000K, 1200K As a benchmark I used the spontaneous ignition temperature form Material Safety Data Sheet (MSDS) to compare my results and real values.

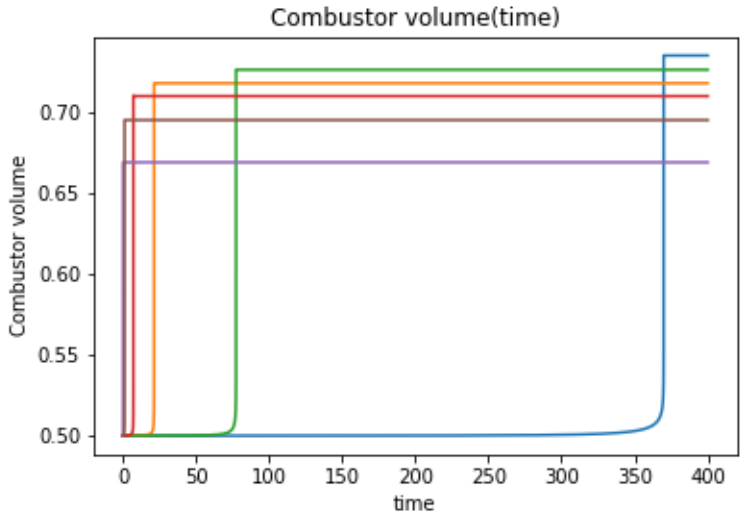
3.1 CH_4



Temperature plot

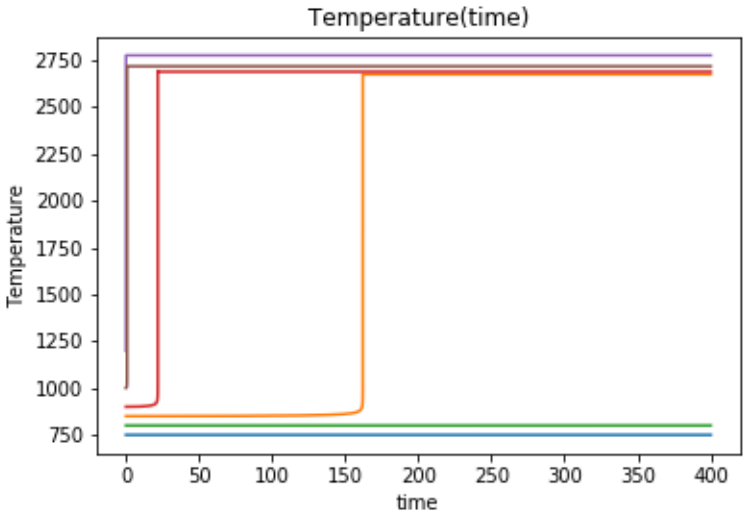


Pressure plot

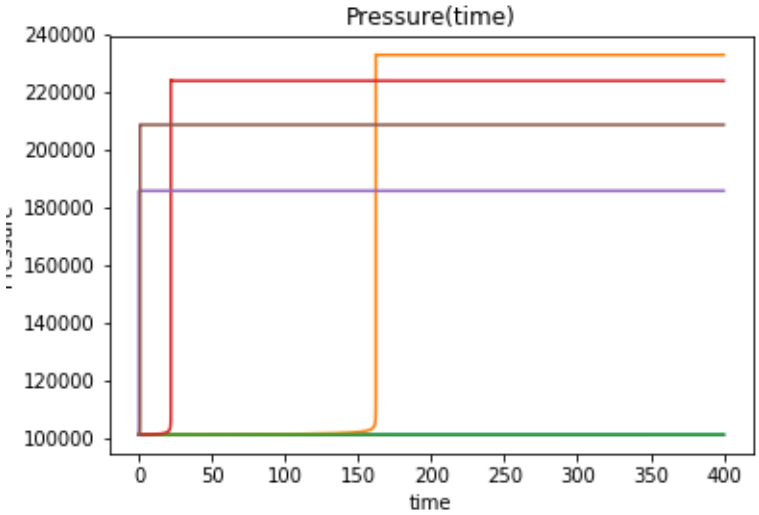


Volume plot

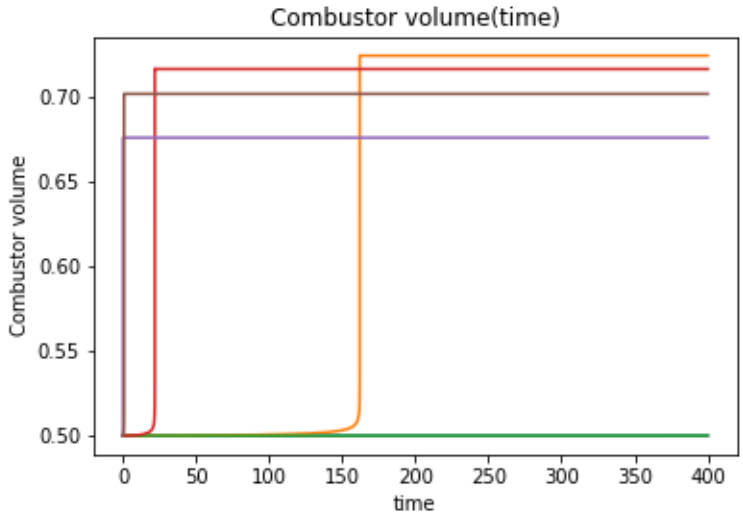
3.2 C_2H_6



Temperature plot

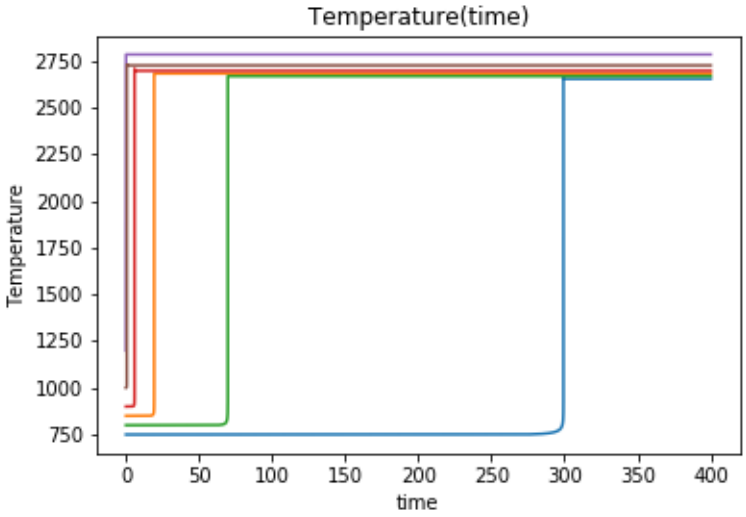


Pressure plot

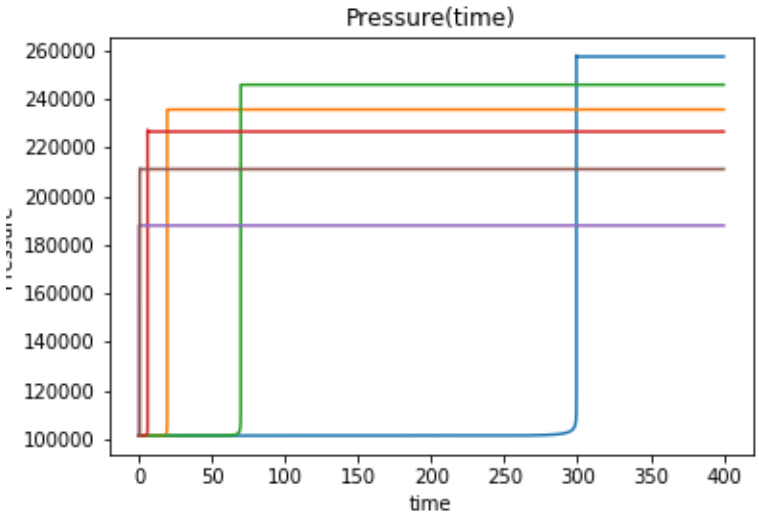


Volume plot

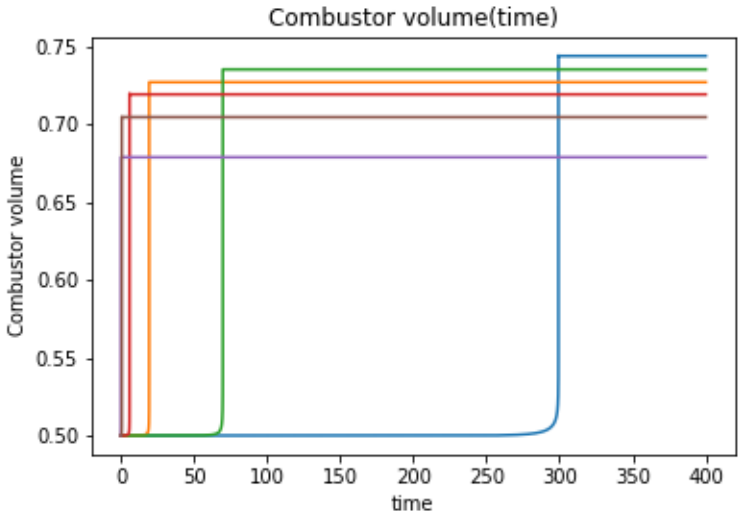
3.3 C_3H_8



Temperature plot



Pressure plot



Volume plot

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. For CH_4 auto-ignition time lasts less than a second and in two other cases it takes hundreds of seconds to spontaneous ignition. 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 C_2H_6 and ca. 850K for C_3H_8, so it is more or less similar to actual values.
Another conclusion is quite simple - 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
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