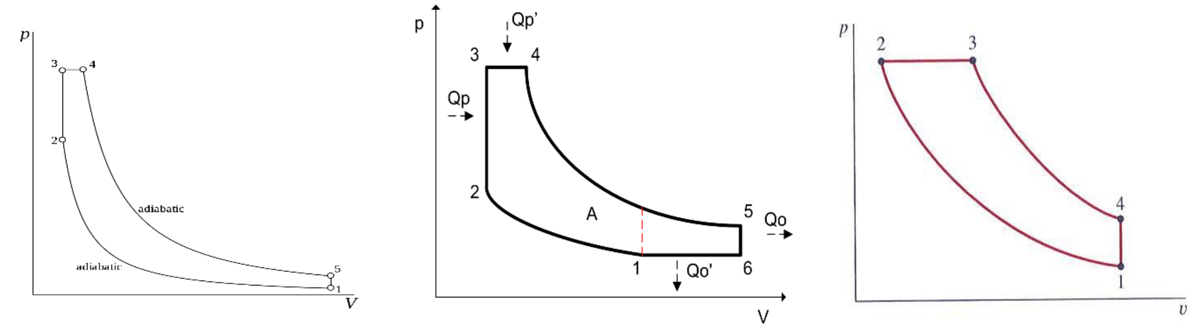
Combustion of an air – propane mixture in a constant volume combustion chamber

(Mathia Fiorelli, LiK, Metody Komputerowe w Spalaniu)

1. Introduction

Combustion in a constant volume chamber is a relatively common phenomenon. It is present in the Sabathe (fig.1), Atkinson (fig. 2) and Diesel (fig3) and gas cycle. It is (theoretically) observed in CI engines, which are growing more popular, especially in the general aviation sector, since the AvGas prices are have gone up. In a Bechtel's document [1] it has been stated that Constant Volume Combustion has the "*highest efficiency approach to reaching the ideal Carnot Cycle"* It is important to fully understand the process, and be able to simulate it, in order to reduce the cost of elaborating and implementing new technologies. This report's purpose is to investigate the influence of different combinations of initial pressure, temperature and concentration of the air – propane solution, on the process of combustion.



Figures 1 - 3 from left to right. Representation of engine cycles on the P – V diagram

2. Mathematical model and code analysis

In order to simulate said combustion, the Cantera software tool was implemented, especially the GRI-Mech 3.0 chemical reaction mechanism. The way it operates is rigorously explained on the GRI – Mech website [2] and other papers published by The University of California, Berkeley, Stanford University, The University of Texas at Austin and SRI international. For the sake of simplicity of this report, the elaboration on how GRI -Mech works is omitted on purpose. Any reader who is interested in the topic is invited to visit the said website. The code written to perform the calculations was based on the one published as an example on the Cantera website [3], called reactor1.py and is present both in this report and in the github repository [4].

At the base of the algorithm lays the declaration of the most important values of the process. Those values are:

- Initial temperature of the solution `temperatura0`
- Initial pressure of the solution `cisnienie0`
- Concentration of propane in relation to air `stezenie1 = 1 / a`

With those three values the volume of the chamber is derived through the general gas equation:

$$volume0 = (1 + 4.76 \cdot a) \cdot B \cdot \frac{temperatura0}{cisnienie0}$$

Where B is the gas constant and approximately equal to $8.314 \frac{J}{mole \cdot kg}$.

Thus the chemical equation will look this way:

$$C_3H_8 + a(O_2 + 3.76N_2) \rightarrow \cdots$$

Results were collected after inserting the solution in the reactor and starting the time (in a specific moment, set by trial and error).

3. Results and discussion

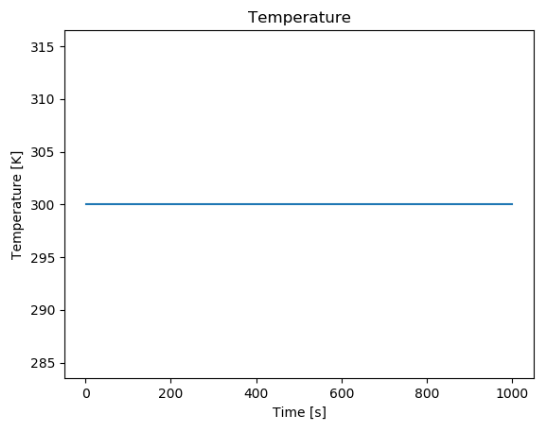
As it was stated before, the aim of this report is try to comprehend the influence of initial pressure, temperature and concentration on the process of combustion in a constant volume chamber. In order to visualize said influence several plots have been generated so the change in time of several chosen variables may be observed. Those variables are:

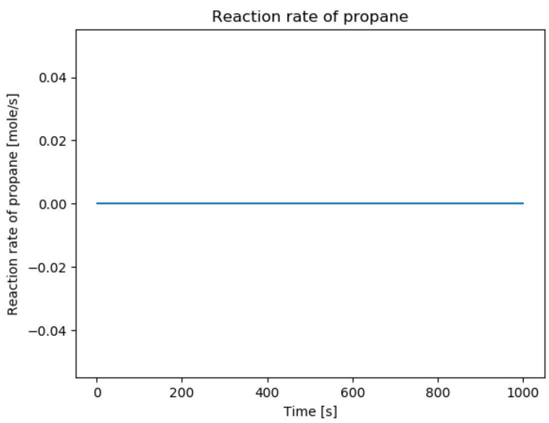
- Temperature
- Pressure
- Rate of reaction

Table 1 Sets of initial values

Set 1			**Set 2**		
Temperature [K]	Pressure [Pa]	Concentration [%]	Temperature [K]	Pressure [Pa]	Concentration [%]
300	10^5	20%	700	10^5	20%
Set3			**Set 4**		
Temperature [K]	Pressure [Pa]	Concentration [%]	Temperature [K]	Pressure [Pa]	Concentration [%]
700	10^8	20%	1000	10^5	20%
Set 5			**Set 6**		
Temperature [K]	Pressure [Pa]	Concentration [%]	Temperature [K]	Pressure [Pa]	Concentration [%]
1000	10^5	5%	1000	10^5	70%

3.1.Set 1

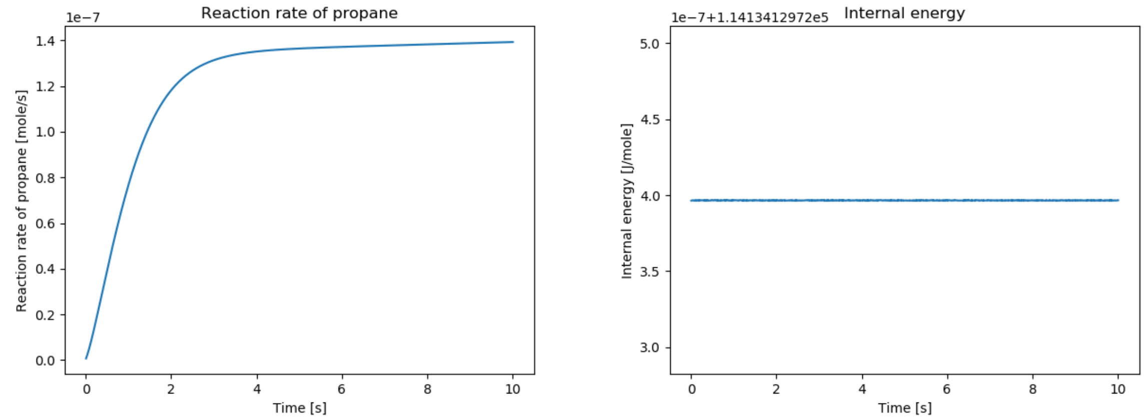




Figures 4 – 6 Set 1 plots

As we can see there is no characteristic spike in temperature nor there's any production rate. There is no reaction in course in these conditions.

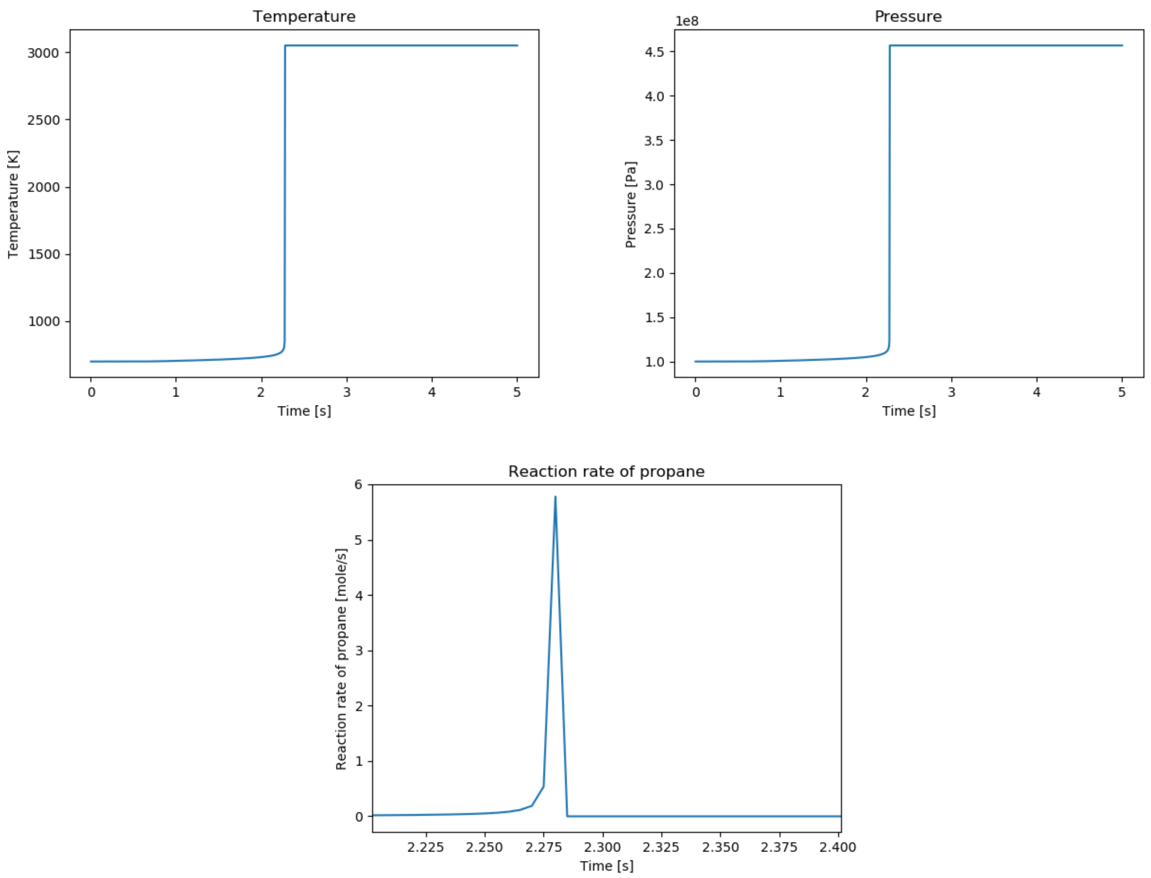
3.2. Set 2



Figures 7 – 8 Set 2 plots

Here we can see that the internal energy is constant, because of that, and of the fact that the reaction takes place in a constant volume reactor, the temperature and pressure are also constant. This reaction is an example of a slow oxidation.

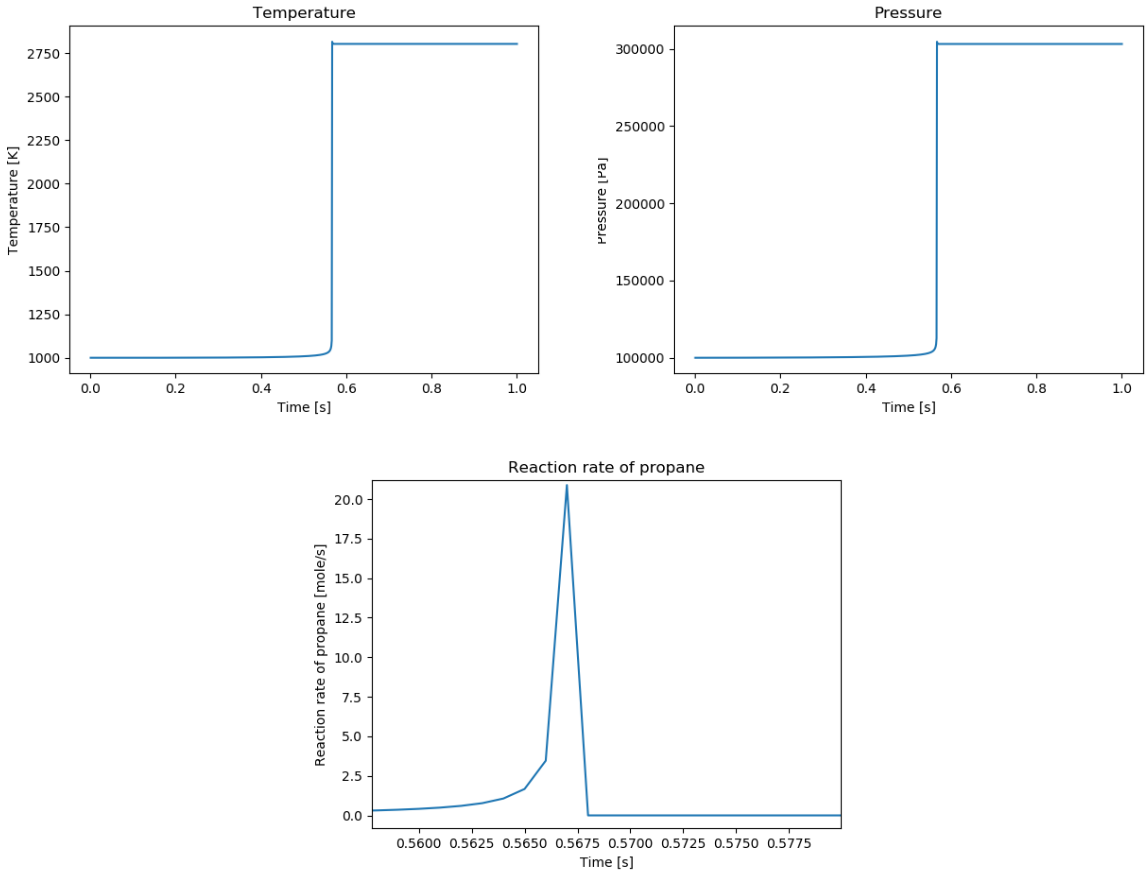
3.3. Set 3



Figures 9 – 11 Set 3 plots

This is an excellent example of the stechiometric process of combustion. We can observe the characteristic spike in all reaction rate, pressure and temperature. The reaction rate, however is relatively low.

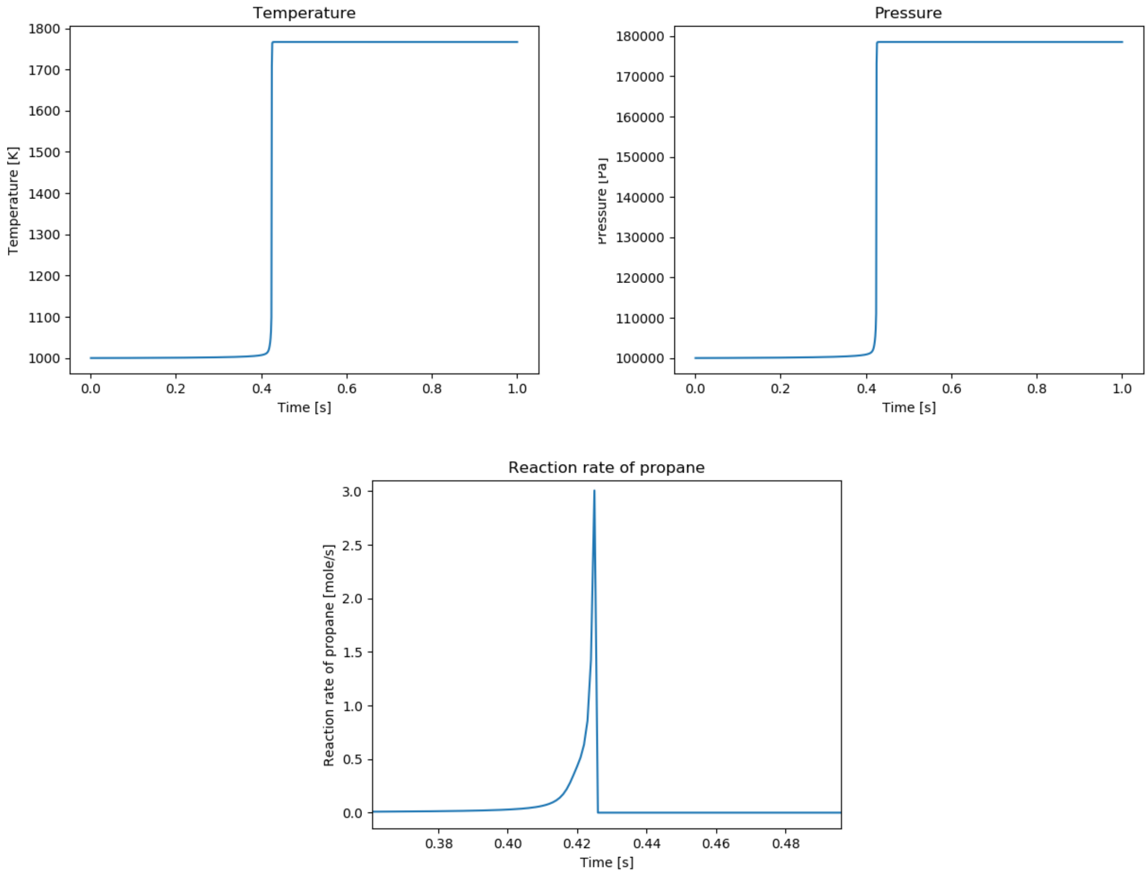
3.4. Set 4



Figures 12 – 14 Set 4 plots

This is also an example of a stechiometric combustion process in a relatively higher temperature. We can see that the reaction rates are higher than in the previous set, but the increase in temperature is not as high.

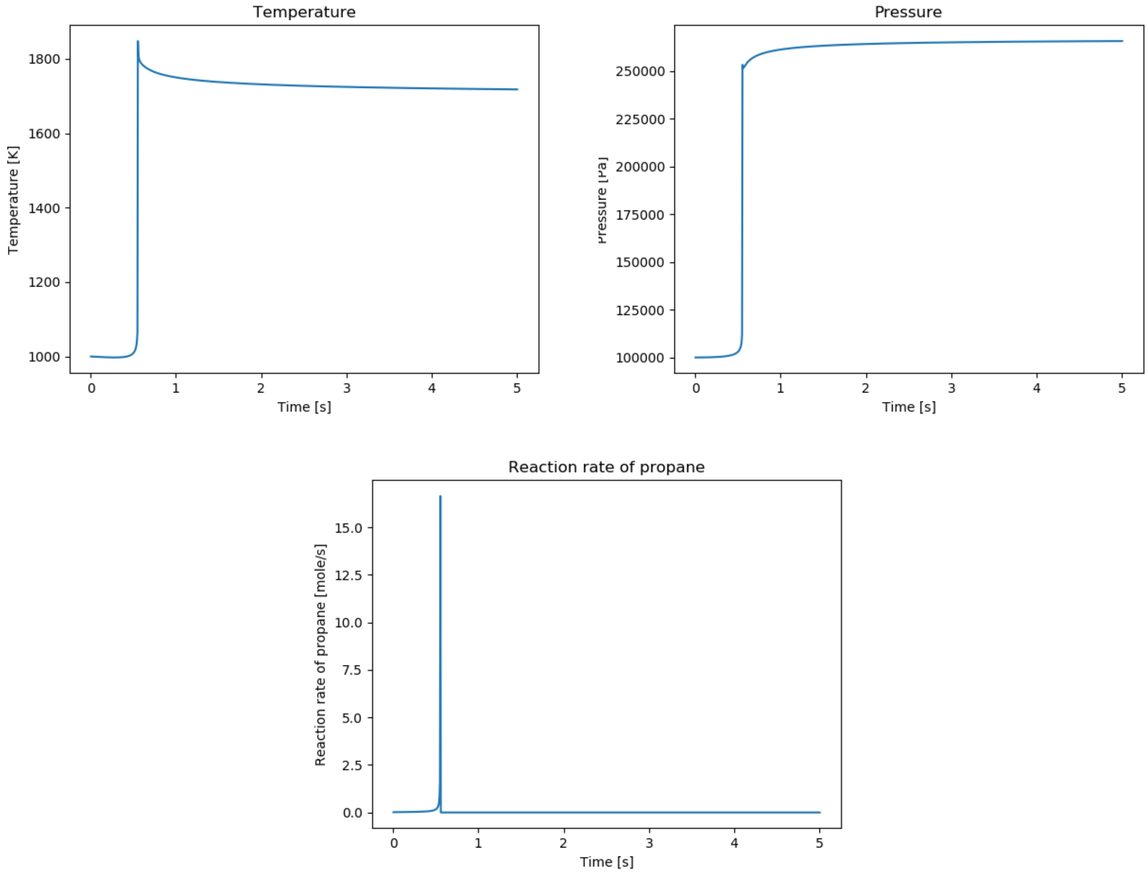
3.5. Set 5



Figures 15 – 17 Set 5 plots

In this set the concentration was lowered, which resulted in a lower increase of all three parameters. It is because the concentration is far from being optimal.

3.6.Set 6



Figures 18 – 20 Set 6 plots

Here the concertation was increased far beyond the optimal one. It resulted in a similar reaction as in the previous set. The temperature plot is similar, however we can observe far greater pressure and reaction rate increase .

4. Conclusions

- Temperature, pressure and concentration have a huge impact on the combustion process in a CVC.
- When the temperature, and pressure are too low combustion may not happen.
- Concentration influences the increase of temperature and pressure and vice versa
- It is possible to ignite the solution not only by temperature but also by pressure

Acknowledgement

Mr. Jakub Majewski, Krystian Pietrzak, and Aleksander Łyczek proved to be immensably helpful during the writing of this project, as their insight helped find errors and operate the software.

5. References

1. S.C. Gulen PhD, PE: *Constant volume combustion: the ultimate gas turbine cycle*
2. GRI – Mech project overview: *http://combustion.berkeley.edu/gri-mech/overview.html*
3. David G. Goodwin, Harry K. Moffat, and Raymond L. Speth. *Cantera: An object- oriented software toolkit for chemical kinetics, thermodynamics, and transport processes.* http://www.cantera.org, 2017. Version 2.3.0. doi:10.5281/zenodo.170284
4. https://en.wikipedia.org/wiki/Atkinson_cycle
5. https://en.wikipedia.org/wiki/Diesel_cycle
6. https://en.wikipedia.org/wiki/Mixed/dual_cycle