Comparison of selected burning properties of various gases in zero-dimensional space in Cantera

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1 Introduction

The aim of this project was to find the self-ignition temperature of various gases in different parameters of temperature and pressure at the start and to compare it and other parameters after the self-ignition using Cantera.

2 Numerical Model

The Cantera Model was based on zero-dimensional reactor filled with gas. The reactor was defined as a ideal gas reactor with constant volume using Cantera function ct.IdealGasReactor. The environment was filled with a heating gas which was a mixture of a hydrogen and an oxygen. There was a wall between the reactor and environment which was a theoretical wall that work was to increase the temperature inside of the reactor. The wall was created with Cantera function ct.Wall.

3 Cases

Differences between each cases were the gas filling the reactor and the value of temperature and pressure of the gas at the start.
There were studied six different gases with three different initial pressures each - 1atm, 10atm and 100atm.
The initial gases temperature was given based on first results given by other Cantera programs. That was done to focus on the most crucial aspect of the process - self-ignition.
The ratio of substrates presumed in the project was taken by the stoichiometry given below.

Methane:
$$CH_4 + 2(O_2 + 3.76N_2) -> CO_2 + 2H_2O + 7.52N_2$$

Ethane:
$$C_2H_6 + 3.5(O_2 + 3.76N_2) -> 2CO_2 + 3H_2O + 13.16N_2$$

Propane:
$$C_3H_8 + 5(O_2 + 3.76N_2) -> 3CO_2 + 4H_2O + 18.8N_2$$

Hydrogen:
$$H_2 + 0.5(O_2 + 3.76N_2) -> H_2O + 1.88N_2$$

$$\text{Methyl alcohol:}$$
$$CH_3OH + 1.5(O_2 + 3.76N_2) -> CO_2 + 2H_2O + 5.64N_2$$

$$\text{Ethylene:}$$
$$C_2H_3 + 3(O_2 + 3.76N_2) -> 2CO_2 + 2H_2O + 11.28N_2$$

4 Results

Results that can be seen in the plots on Figures 1-18, show, that in every case there was a significant increase of parameters of the gas after it received necessary amount of energy.
The self-ignition process requires lower amount of energy for higher initial pressure which is equal to lower self-ignition temperature and overall temperature.
Linear value change of specific internal energy is a result of constant flow of heat through the wall.

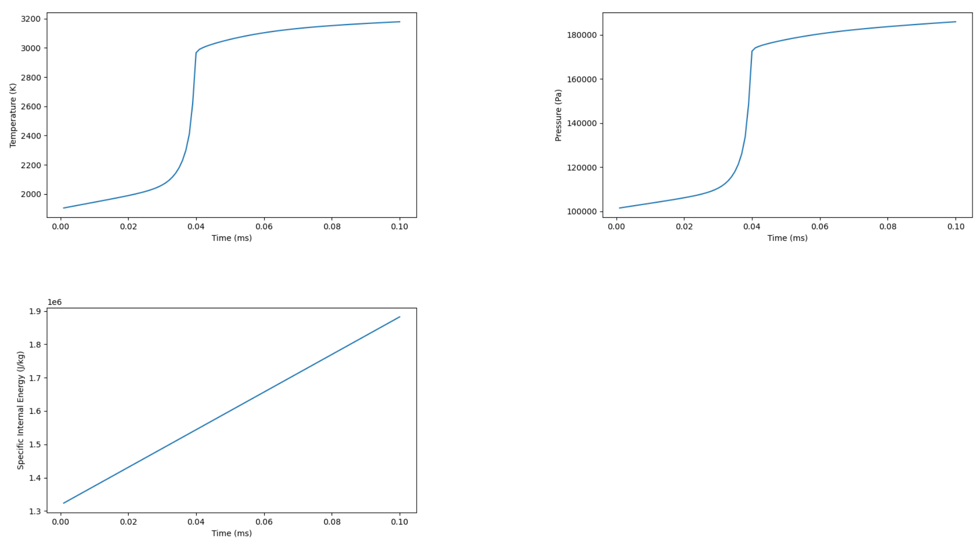

Figure 1: Plots of methane in pressure 1atm at start

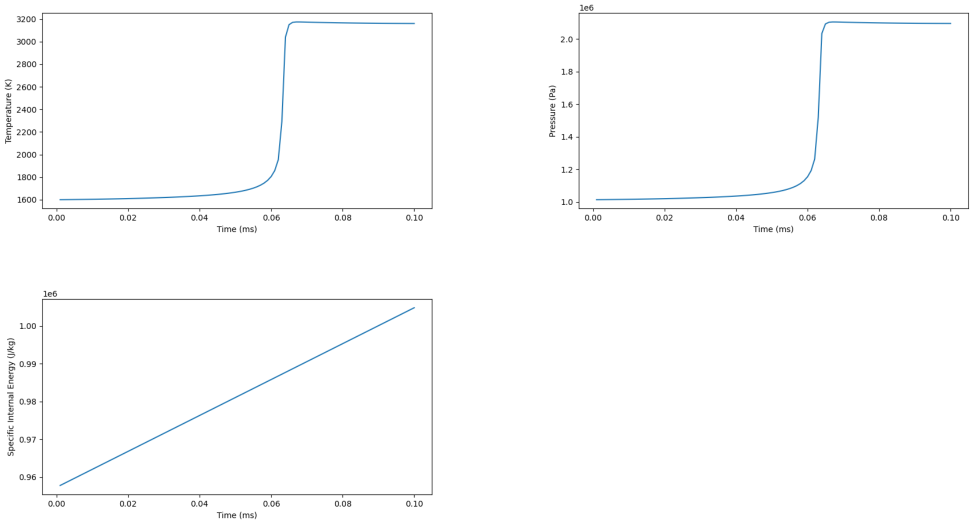

Figure 2: Plots of methane in pressure 10atm at start

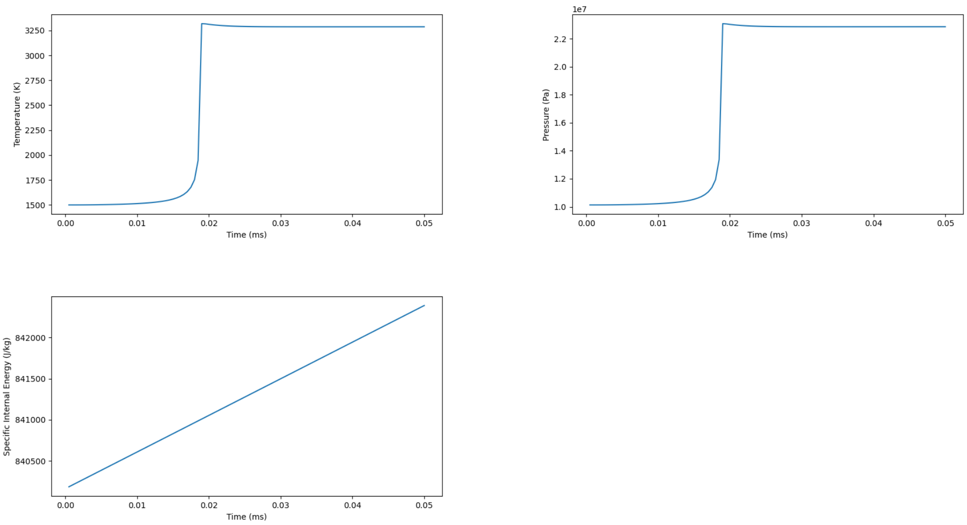

Figure 3: Plots of methane in pressure 100atm at start

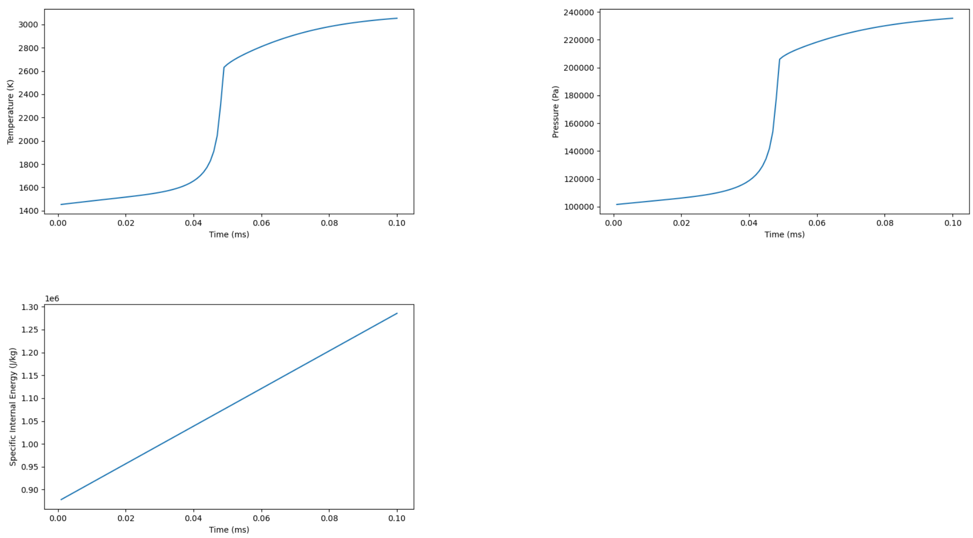

Figure 4: Plots of ethane in pressure 1atm at start

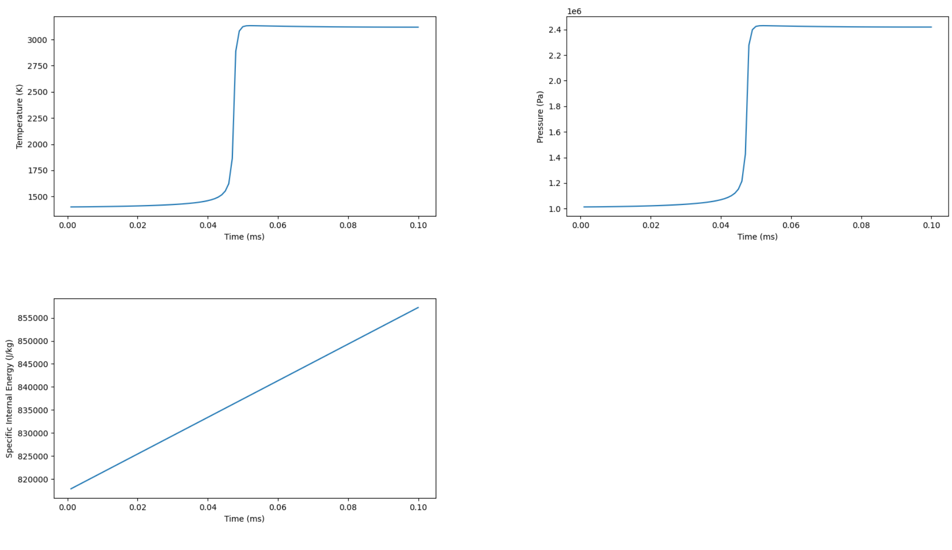

Figure 5: Plots of ethane in pressure 10atm at start

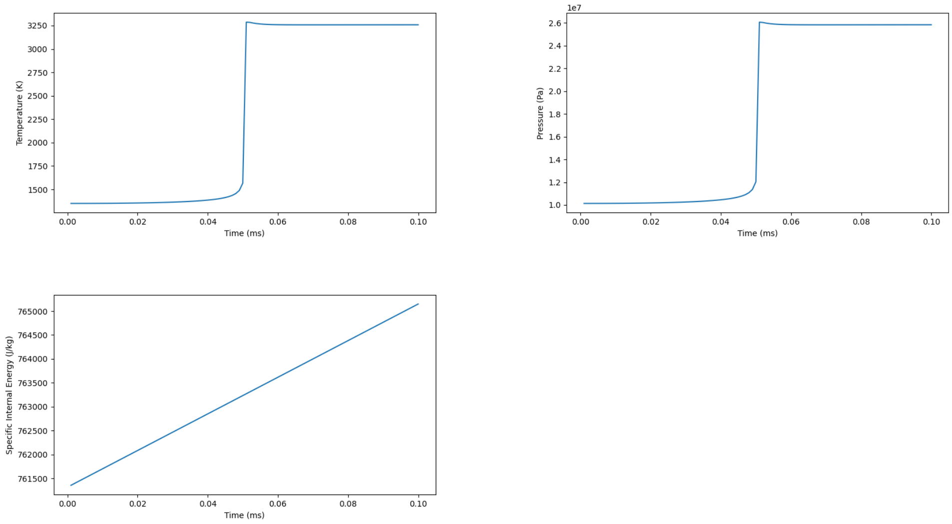

Figure 6: Plots of ethane in pressure 100atm at start

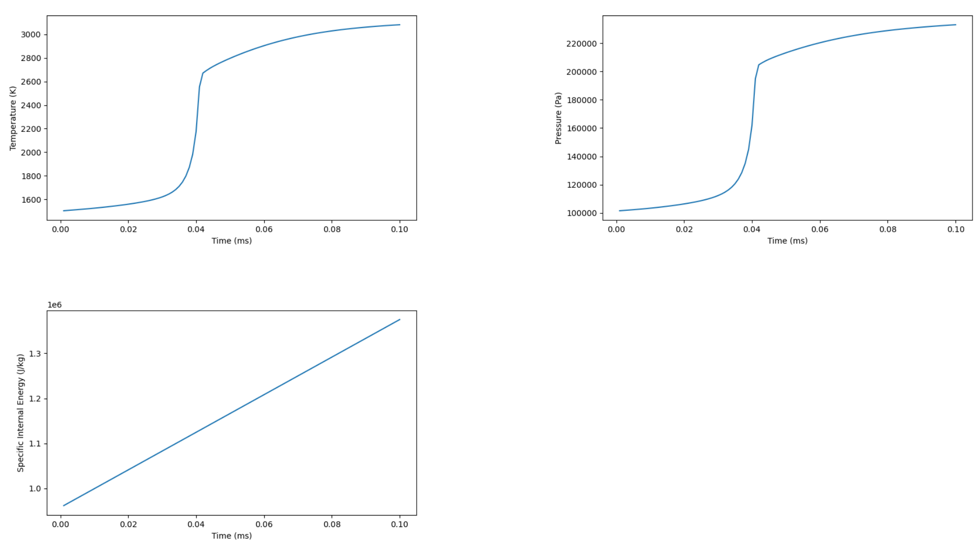

Figure 7: Plots of propane in pressure 1atm at start

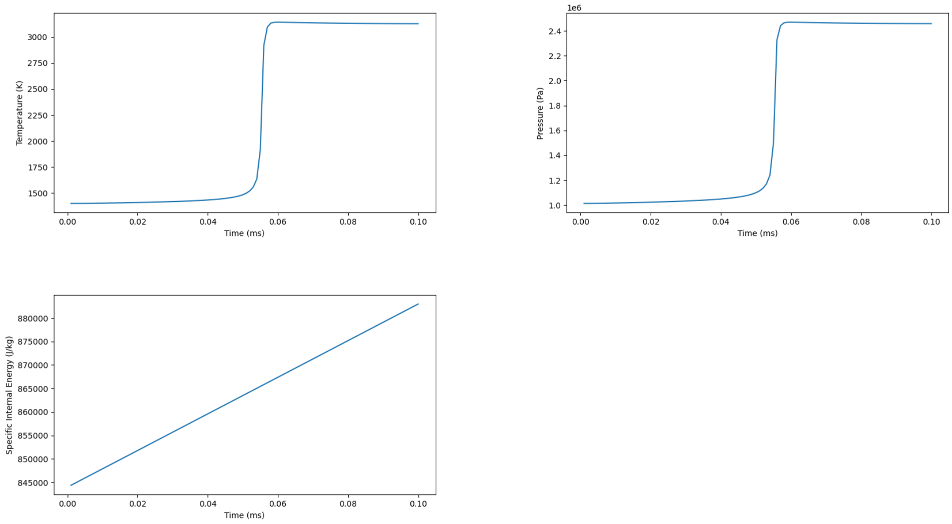

Figure 8: Plots of propane in pressure 10atm at start

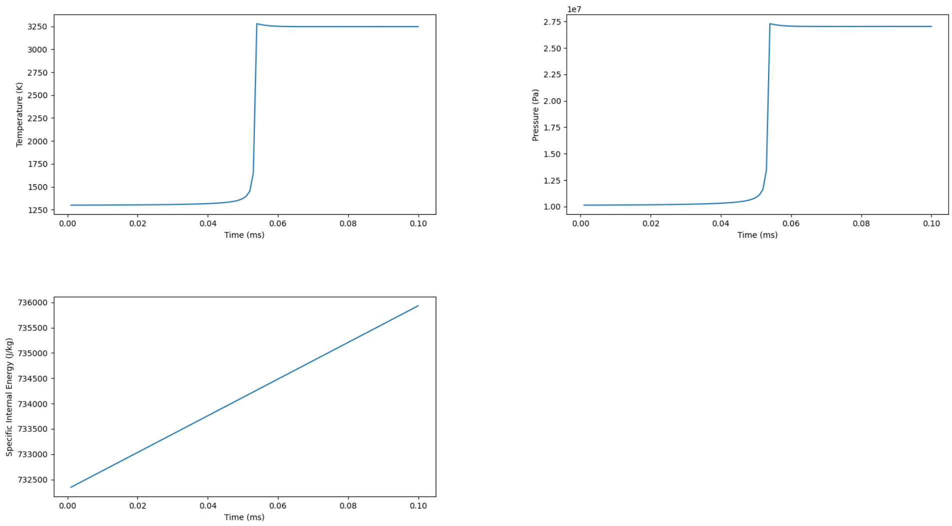

Figure 9: Plots of propane in pressure 100atm at start

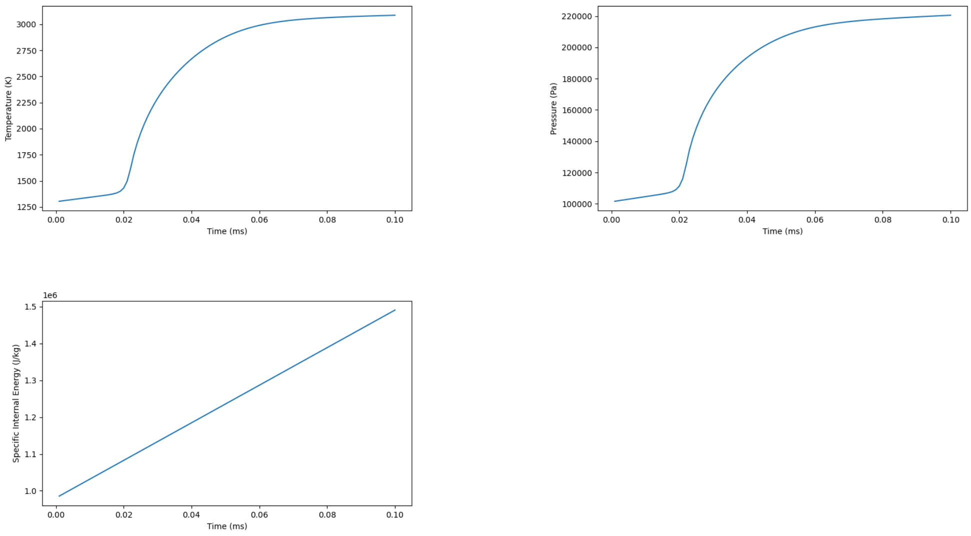

Figure 10: Plots of hydrogen in pressure 1atm at start

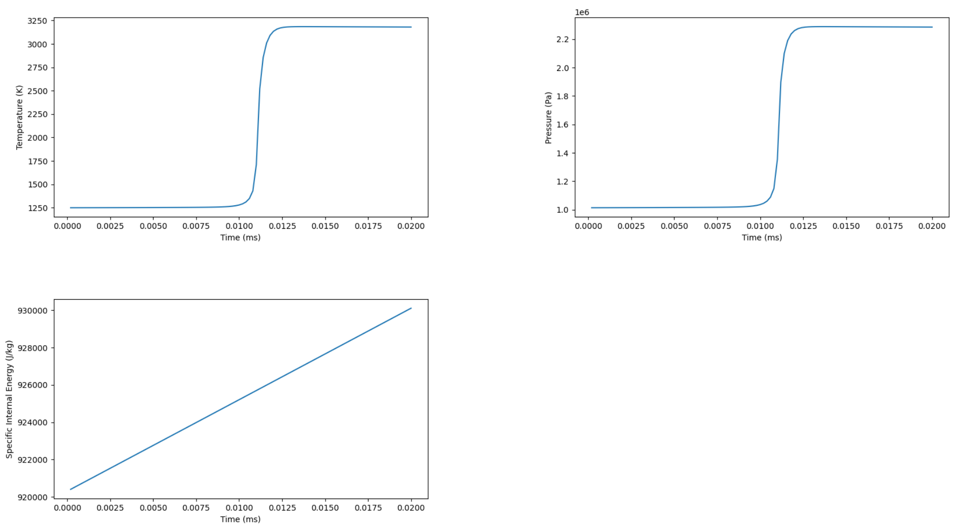

Figure 11: Plots of hydrogen in pressure 10atm at start

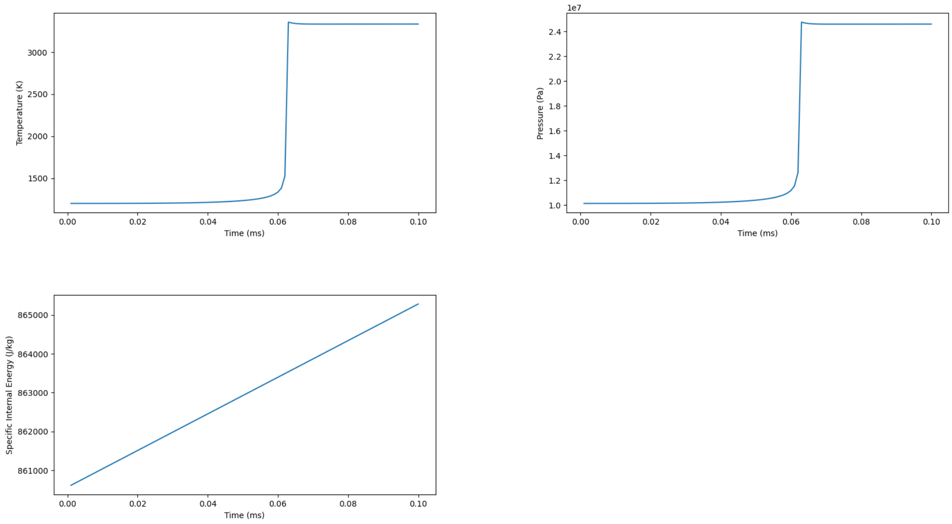

Figure 12: Plots of hydrogen in pressure 100atm at start

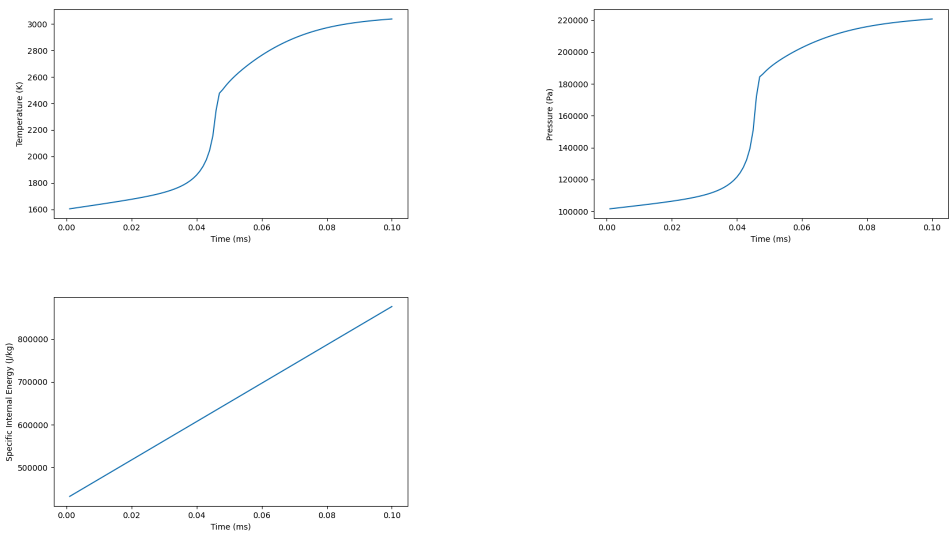

Figure 13: Plots of methyl alcohol in pressure 1atm at start

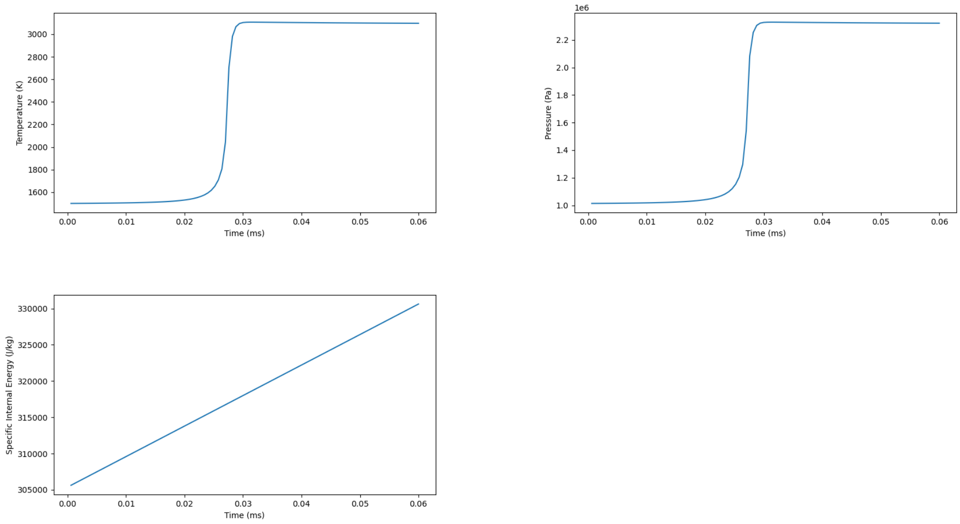

Figure 14: Plots of methyl alcohol in pressure 10atm at start

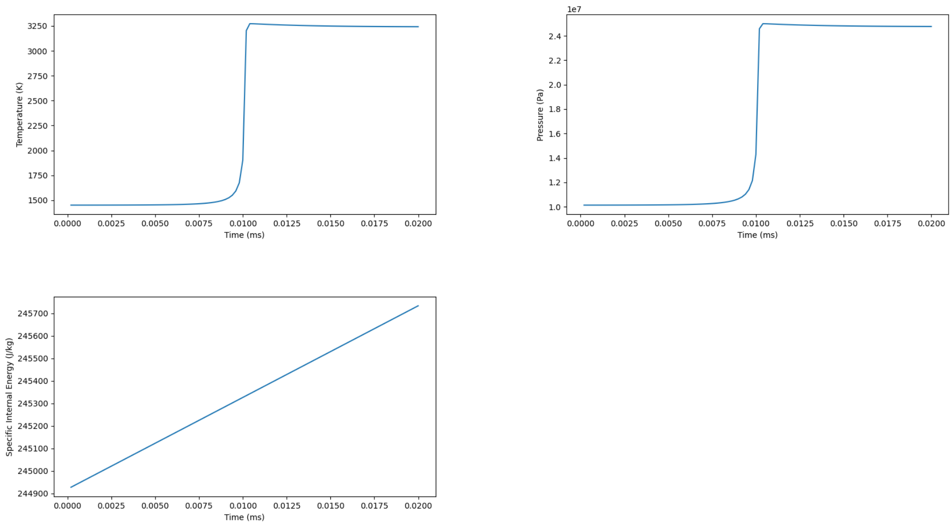

Figure 15: Plots of methyl alcohol in pressure 100atm at start

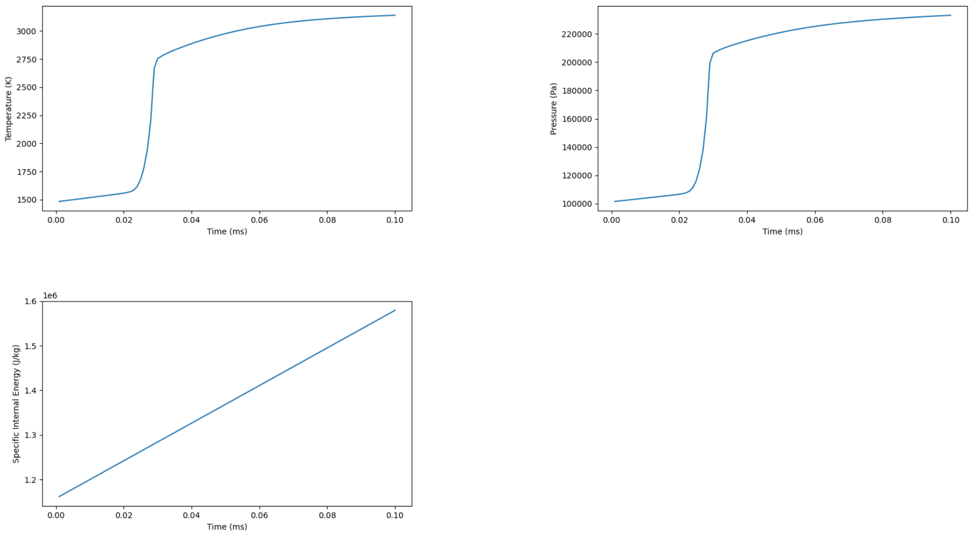

Figure 16: Plots of ethylene in pressure 1atm at start

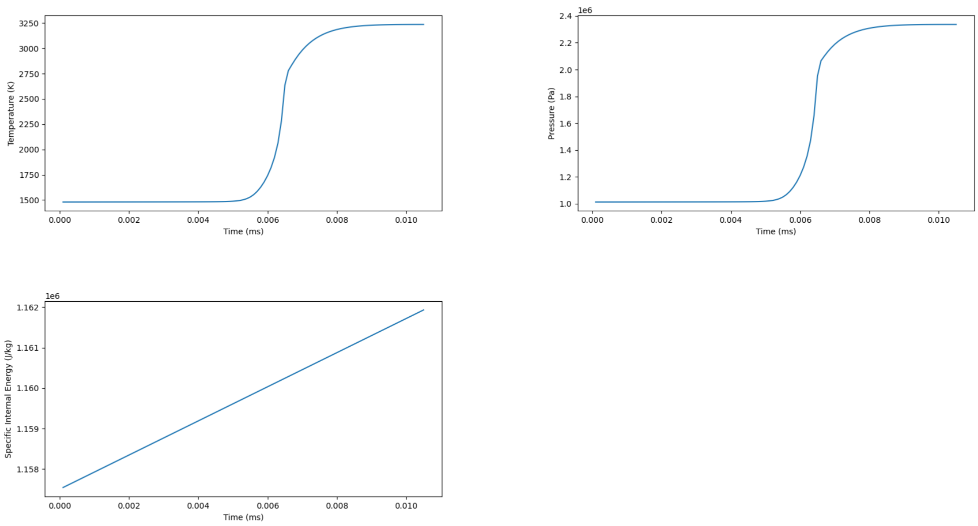

Figure 17: Plots of ethylene in pressure 10atm at start

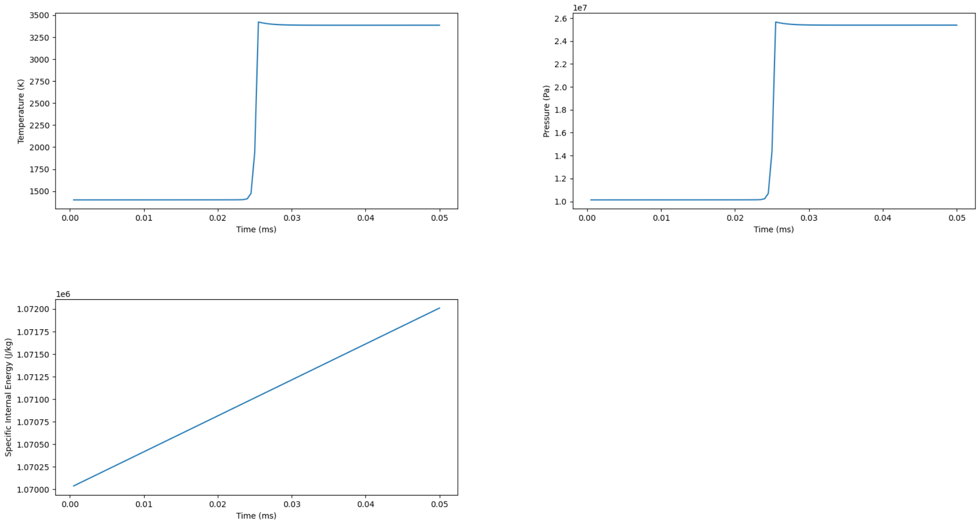

Figure 18: Plots of ethylene in pressure 100atm at start

5 Conclusion

There is a significant difference between results of this experiment and values known from other sources. The differences can exist because of many reasons, including some assumptions made in the start such as existing of ideal gas reactor or stoichiometry. However, the main problem of this experiment is a Cantera Model which probably has not been done correctly, since it gives no quantitative data in comparison to reality, still it delivers some qualitative results and a basic knowledge of using Cantera.

6 Sources

1. https://cantera.org/examples/python/reactors/reactor1.py.html (06.06.2020)
2. https://cantera.org/examples/python/reactors/reactor2.py.html?fbclid=IwAR1RtBiH5h1BC0lIdEAQvLR309lA1 lcRHI (06.06.2020)
3. https://cantera.org/documentation/docs-2.4/sphinx/html/cython/thermo.html (09.06.2020)
4. https://cantera.org/documentation/docs-2.4/sphinx/html/cython/zerodim.html (09.06.2020)
5. https://royalsocietypublishing.org/doi/pdf/10.1098/rspa.1937.0102 (10.06.2020)
6. https://www.engineeringtoolbox.com/ (10.06.2020)
7. http://www.cerfacs.fr/cantera/docs/tutorials/tutoreactors.pdf (10.06.2020)
8. https://www.pythonforbeginners.com/