Politechnika Warszawska

Wydział Mechaniczny Energetyki i Lotnictwa

Metody Komputerowe w Spalaniu

Parameters of hydrogen detonation in SDToolbox

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1 Introduction

Subject of this project is to evaluate parameters such as temperature, pressure and Chapman-Jouguet speed after detonation. CJ speed is velocity of propagation shock wave.

2 Model description

2.1 Software

To solve this problem i used Cantera which was written in C++, and could be used with C++, Python, Matlab and Fortran. I used Python. And SDToolbox employ Cantera software for the chemistry functionality.

2.2 Gas model

Model using gas was changing by pressure, temperature and concentration. Firstly concentration was variable, pressure was one atmosphere, and temperature was 300K. Secondly initial pressure was variable, concentration was 33% it is concentration of maximum pressure and temperature was 300K. Last step was variable temperature in the same conditions. Detonating gas was hydrogen in the air. Limits of flammability was 20-80%.

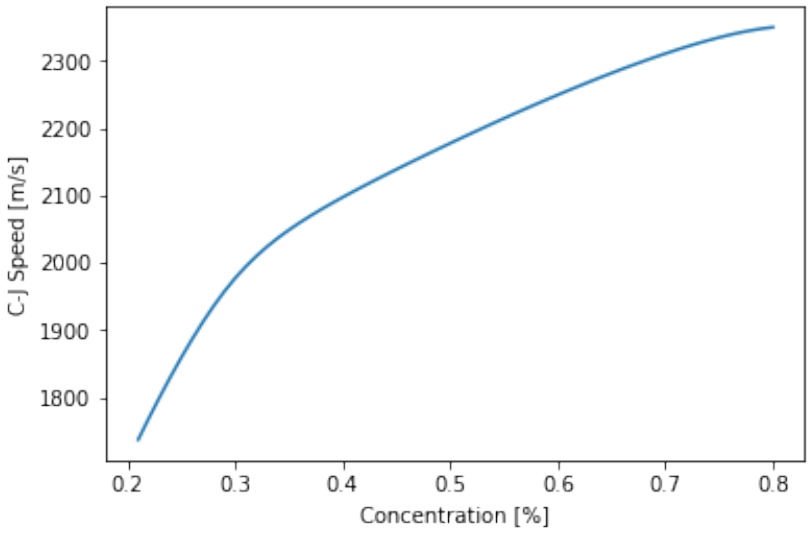
2.3 Activities

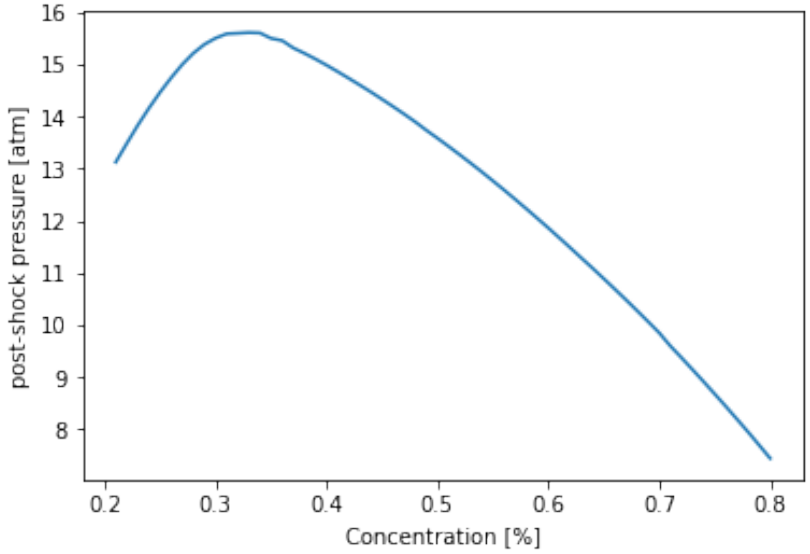
Library of SDToolbox allows user to count gas parameters after shock wave. Initial conditions as pressure, temperature and chemical composition. In code there are three loops iterating thru pressure, temperature and concentration of initial state.

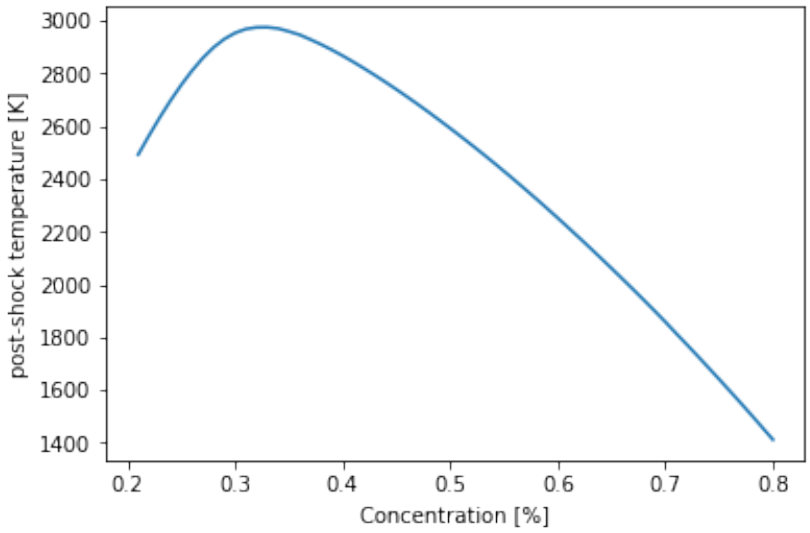
3 Results

I made 9 plots show parameters after shock wave and CJ speed with different starting conditions. I checked in which concentration of hydrogen occures the bigest pressure, and I used it to every other calculation than iterating thru concentrations.

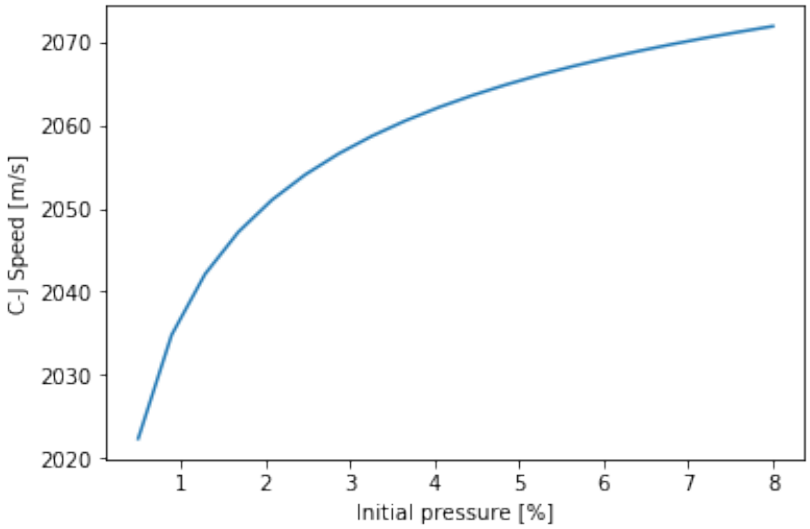
3.1 Variable initial concentration:

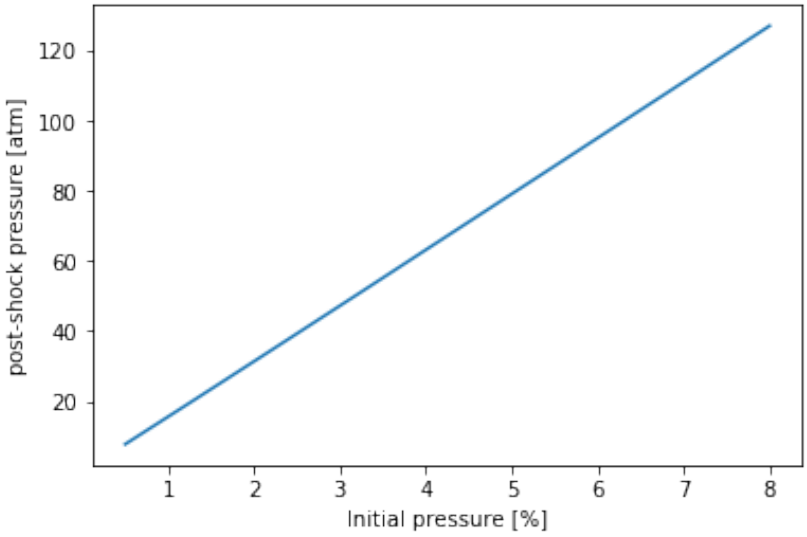


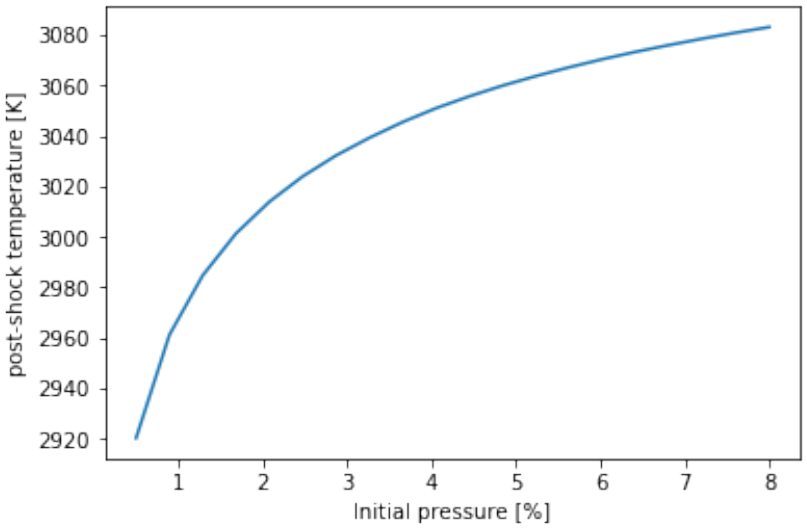




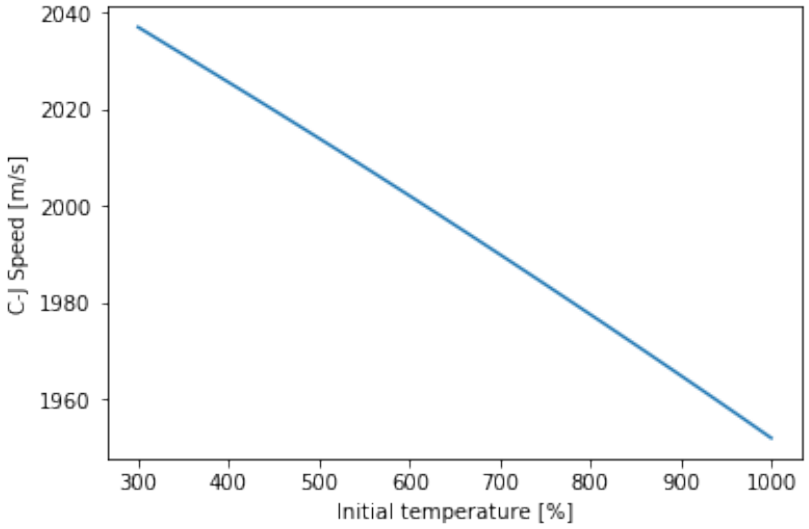
3.2 Variable initial pressure:

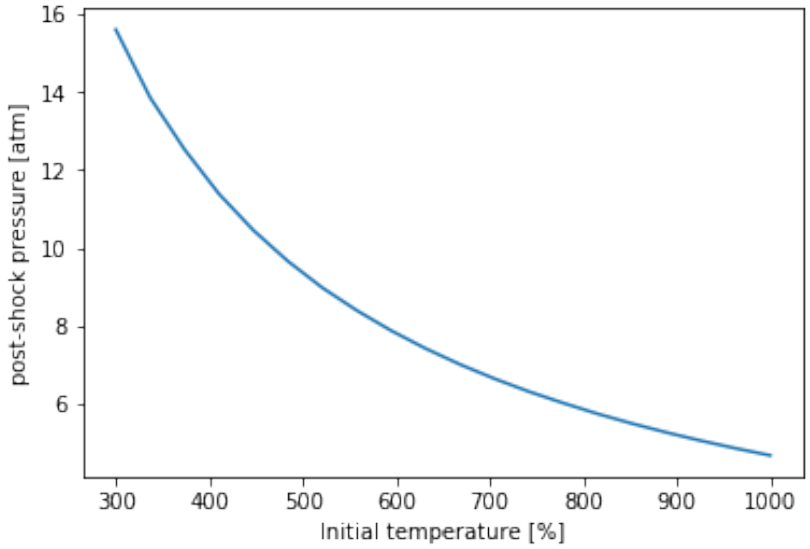


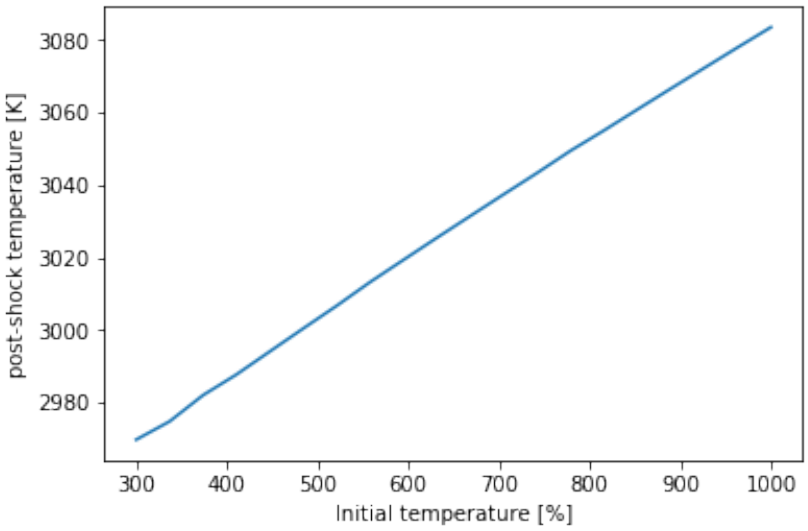

post-shock pressure [atm]
120
100
80
60
40
20
1
2
3
4
5
6
7
8
Initial pressure [%]


post-shock temperature [K]
3080
3060
3040
3020
3000
2980
2960
2940
2920
1
2
3
4
5
6
7
8
Initial pressure [%]

3.3 Variable initial temperature:







4 Conclusion

We can see that post-shock temperature and pressure depends respectively linearly from initial temperature and pressure. The highest pressure, and highest temperature we accomplish in the same concentration of hydrogen. Speed is rising with concentration and pressure and falls with temperature.

5 Bibliography

MKWS lectures
SDToolbox demos