Politechnika Warszawska

Wydział Mechaniczny Energetyki i Lotnictwa

Metody Komputerowe w Spalaniu

Parameters of hydrogen detonation in SDToolbox

Author:
Małgorzata Stokowska

Supervisor:
Dr. Mateusz Żbikowski

June 27, 2018

1 Introduction

Subject of this project is to evaluate parameters such as temperature, pressure and Chapman-Jouguet speed after detonation. The Chapman–Jouguet condition holds approximately in detonation waves in high explosives. It states that the detonation propagates at a velocity at which the reacting gases just reach sonic velocity (in the frame of the leading shock wave) as the reaction ceases. David Chapman and Émile Jouguet originally stated the condition for an infinitesimally thin detonation.

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 SD-Toolbox employ Cantera software for the chemistry functionality. The Shock & Detonation Toolbox is a collection of numerical routines that enables the solution of standard problems for gas-phase explosions using realistic thermochemistry and detailed chemical kinetics. It is possible to use SDTolbox for:

- CJ detonation speed and post-detonation state
- Postshock gas state for frozen composition
- Postshock gas state for equilibrium composition
- Frozen and equilibrium Hugoniot curves
- Constant-volume explosion structure
- ZND detonation structure
- Effective activation energies and chemical time scales from detailed reaction mechanisms
- Extrapolation of low temperature thermodynamic polynomial fits to higher temperatures.

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%. The GRI-Mech 3.0 chemical reaction mechanism was used.

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.
This is the most important part of the code:

- CJspeed(P1, T1, X, mech, 0) - computation of CJ speed
- PostShock_eq(cj_speed, P1, T1, X, mech) - computaton of the post shock state
- T2.append(gas.T) - appending to a list of post shock temperature
- P2.append(gas.P/one_atm) - appending to a list of post shock pressure
- speed.append(cj_speed) - appending to a list of CJ speed

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.

1. Initial conditions 300K, one atmosphere
2. Initial conditions 300K, 33% concentration of hydrogen
3. Initial conditions ne atmosphere, 33% concentration of hydrogen

3.1 Variable initial concentration:

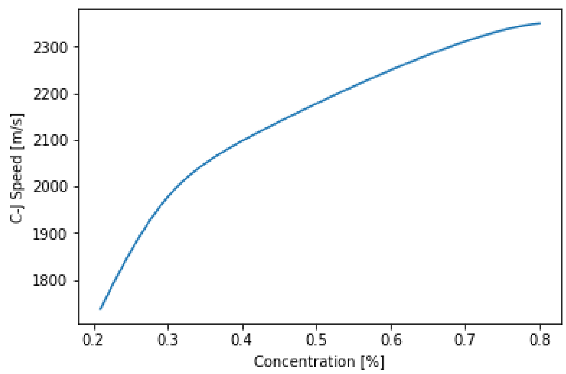

Fig. 1 CJ speed with variable concentration

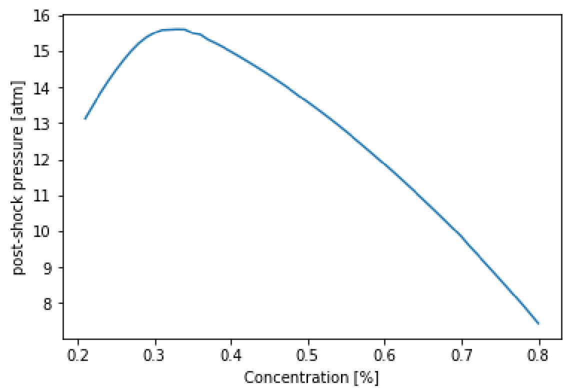

Fig. 2 Pressure with variable concentration

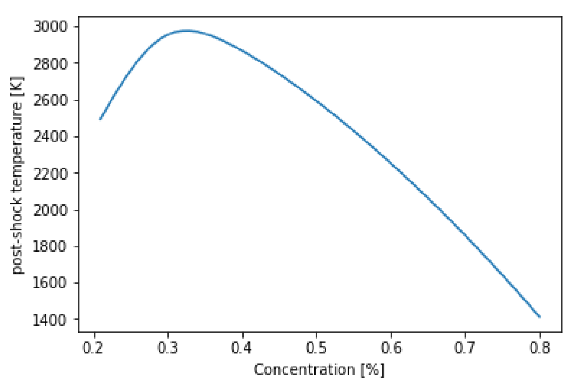

Fig. 3 Temperature with variable concentration

3.2 Variable initial pressure:

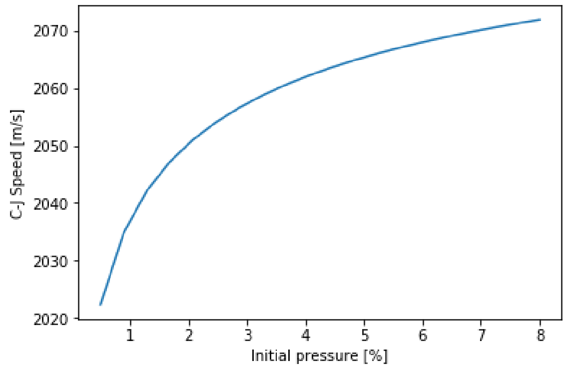

Fig. 4 CJ speed with variable pressure

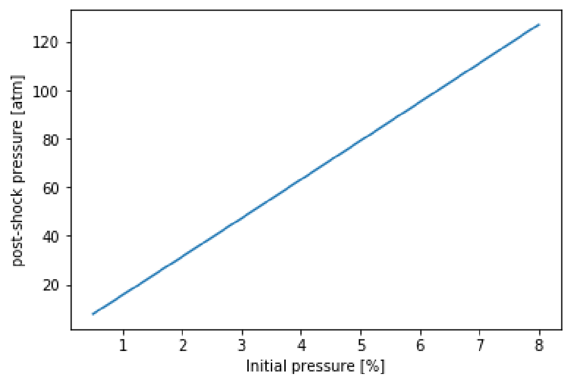

Fig. 5 Pressure with variable pressure

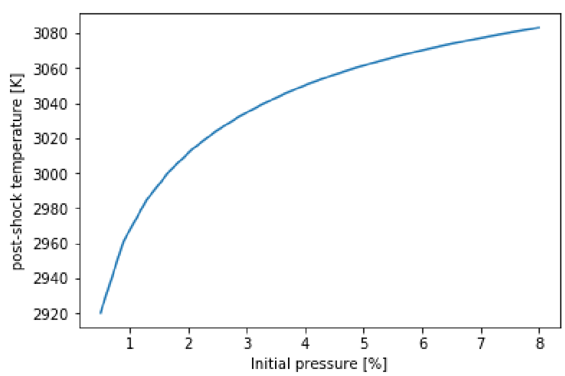

Fig. 6 Temperature with variable pressure

3.3 Variable initial temperature:

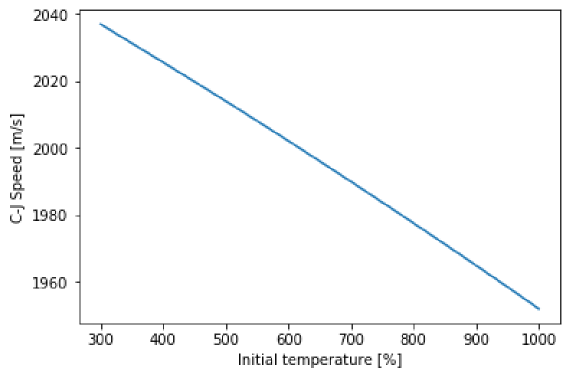

Fig. 7 CJ speed with variable temperature

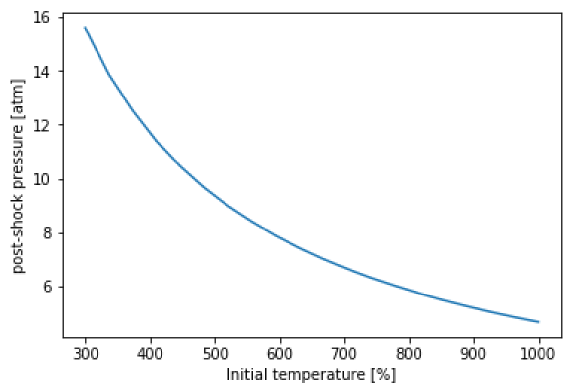

Fig. 8 Pressure with variable temperature

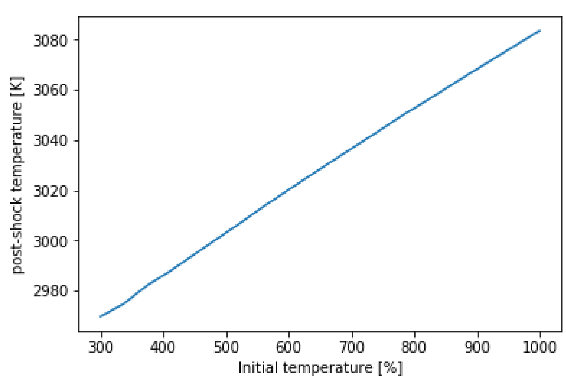

Fig. 9 Temperature with variable temperature

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. Pressure and temperature rise with fuel increasing until stoichiometric when it start falling.
With initial temperature increasing C-J speed and post shock pressure is falling down, but post shock temperature is rising.
To reduce Chapman-Jouguet speed we should increase initial temperature and decrease initial pressure.

5 Bibliography

MKWS lectures
SDToolbox demos