Politechnika Warszawska

Wydzial Mechaniczny Energetyki i Lotnictwa

Metody Komputerowe w Spalaniu

Methane and Hydrogen CJ Speed comparison

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1 Introduction

Subject of this project is to calculate 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 have used Cantera in Python environment. Also SD-Toolbox which employs Cantera software for the chemistry functionality was used. The Shock and 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 had a variable temperature and pressure. Detonating gases were stoichiometric mixtures of hydrogen and methane in the air. The GRI-Mech 3.0 chemical reaction mechanism was used.

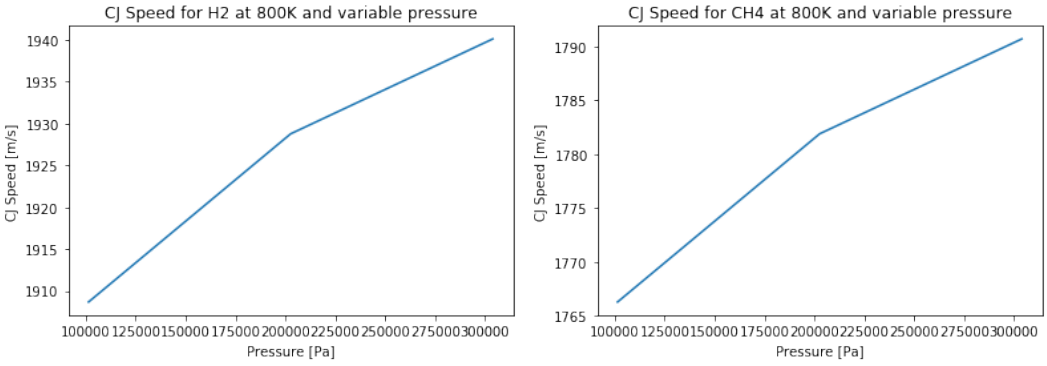
2.3 Actions

Temperature and pressure can be changed in the code. There are set three different pressures for each temperature.

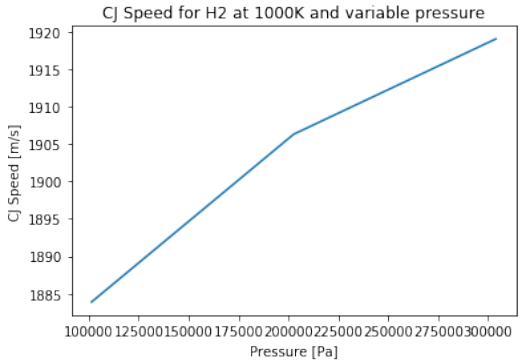
2.4 Results

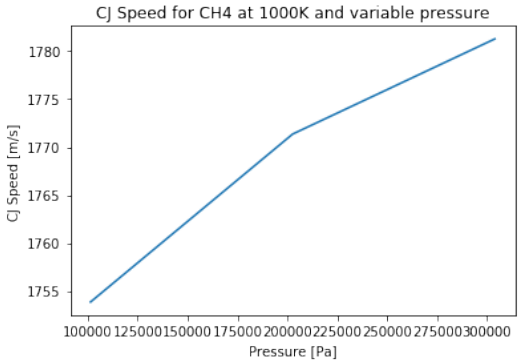
CJ Speeds were computed for three starting temperatures and for three pressures respectively: 800K, 1000K, 1200K and one atm, two atm and three atm for both gases.

2.4.1 800K

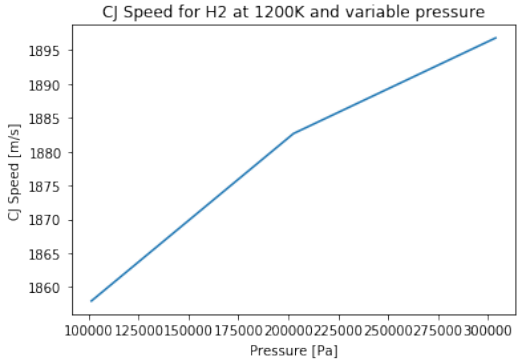


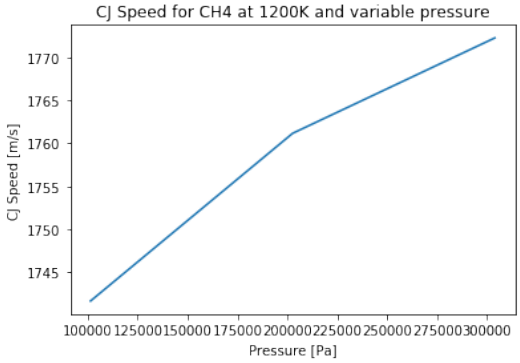
2.4.2 1000K





2.4.3 1200K





3 Conclusion

As can be seen the CJ Speed depends as well well on temperature as on pressure. The higher pressure the faster the reaction is. The Same thing can not be said about temperature, the higher starting temperature the slower the CJ Speed is. What is also noticeable is fact that hydrogen reacts much faster and has quicker CJ Speed in all considered conditions. To reduce Chapman-Jouguet speed we should increase initial temperature and decrease initial pressure.

4 Bibliography

- MKWS lectures
- Cantera website
- Overleaf website
- SDToolbox website