COMPUTIONAL METHODS IN COMBUSTION

Detonation of ethane - oxygen mixture for different initial temperature, pressure and equivalence ratio

Dorota Surowiec
271348

Aerospace Engineering

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1 Introduction

The purpose of the project was to conduct a study of Chapman-Jouguet detonation of a ethane oxygen mixture for different initial temperature, pressure and equivalent ratio, using Cantera and SDToolbox software. The results of the study are several plots, showing influence of these parameters on C-J detonation speed, temperature, pressure and density.

2 Mathematic model

There are several mechanisms that can be used for C-J detonation parameters. For the needs of the study, we used the one called "gri30_highT Mechanism".
The stoichiometric reaction of complete combustion of ethane in oxygen is as follows

$$C_2H_6 + 3,5O_2 \rightarrow 2CO_2 + 3H_2O$$

From the equations of conservation, jump conditions for a detonation are:

$$P_2 = P_1 + \rho\omega_1^2(1 - \frac{\rho_1}{\rho_2})$$

$$h_2 = h_1 + \frac{1}{2}\omega_1^2(1 - (\frac{\rho_1}{\rho_2})^2)$$

The Rayleigh line is a consequence of combining the mass and momentum conservation relations:

$$P_2 = P_1 - \rho_1^2\omega_1^2(v_2 - v_1)$$

Eliminating the post-shock velocity, energy conservation can be rewritten as a purely thermodynamic relation known as the Hugoniot or shock adiabat.

$$h_2 - h_1 = \frac{(P_2 - P_1)(v_2 + v_1)}{2}$$

The minimum wave speed occurs when Reyleigh line is tangent to the Hugoniot. The point of tangency is referred to as the CJ state (Figure 1).
From the coordinates of this point we can get information about the pressure and tem- perature after detonation.

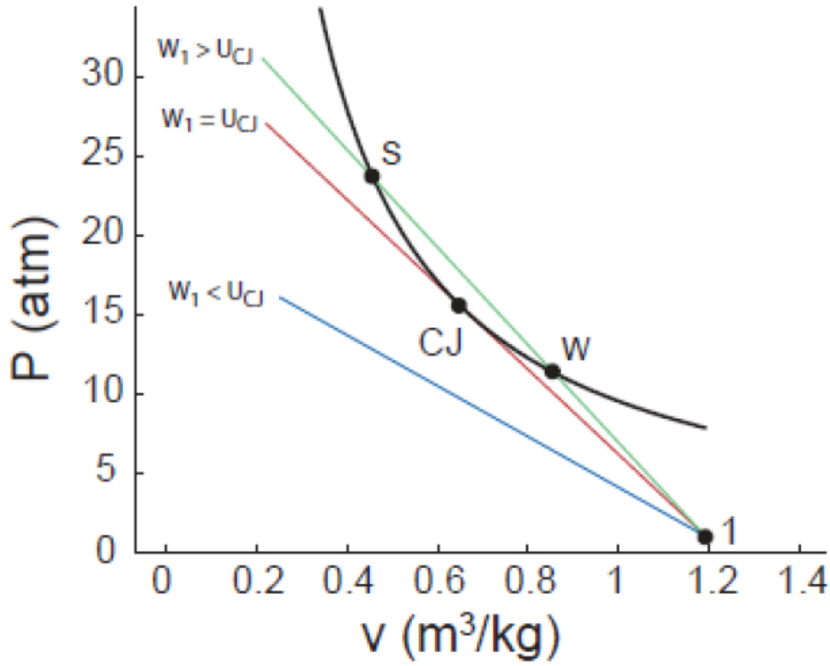

Figure 1: Rayleigh and Hugoniot lines.

The calculations were held for 10 different temperatures, pressures and 11 different values of ϕ(10x10x11). It took couple of minutes to calculate it. The more accurate we want the calculations to be, the more iterations we have to make and the more time it takes. For the purpose of this project, 10x10x11 is more than enough.

3 Results and plots

3.1 Results for $P = 1013,25 hPa$, $\phi = 1$ and different initial temperatures.

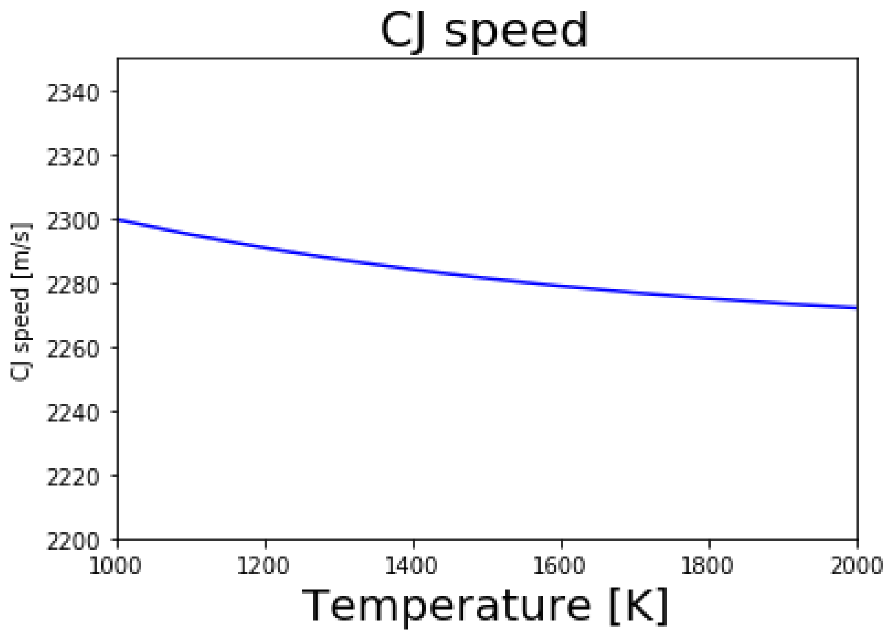

Figure 2: Influence of initial temperature on C-J detonation speed.

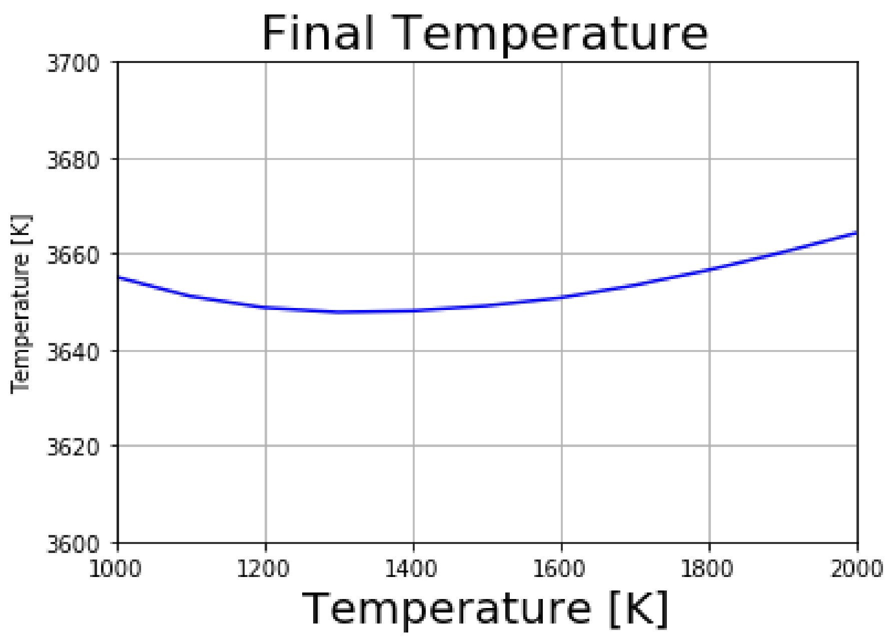

Figure 3: Influence of initial temperature on detonation temperature.

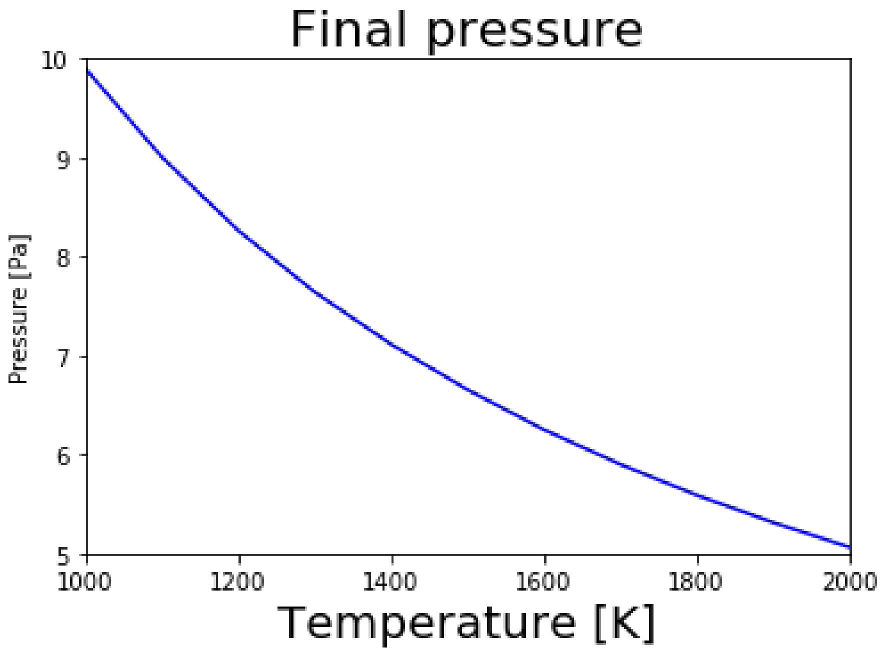

Figure 4: Influence of initial temperature on detonation pressure.

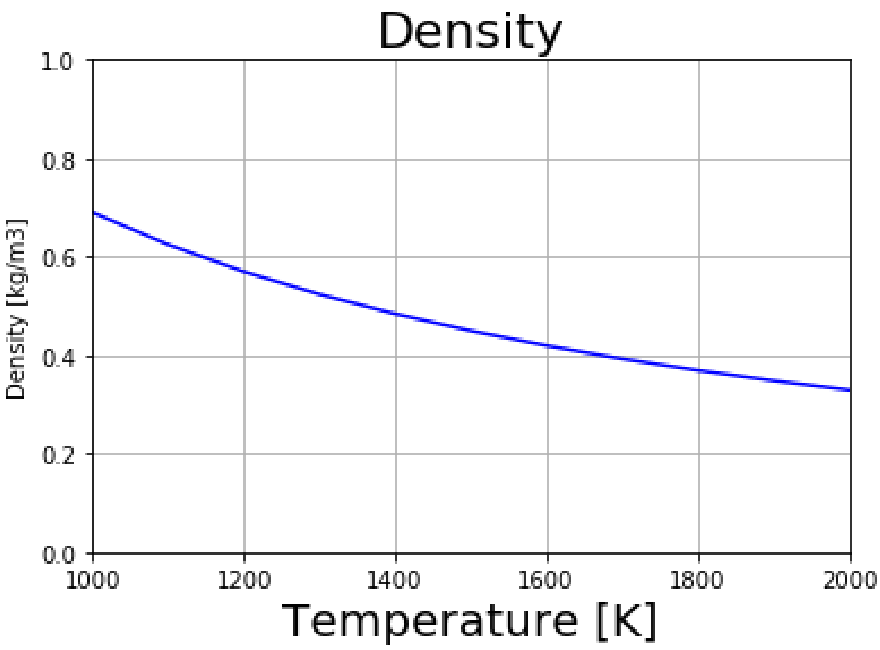

Figure 5: Influence of initial temperature on detonation density.

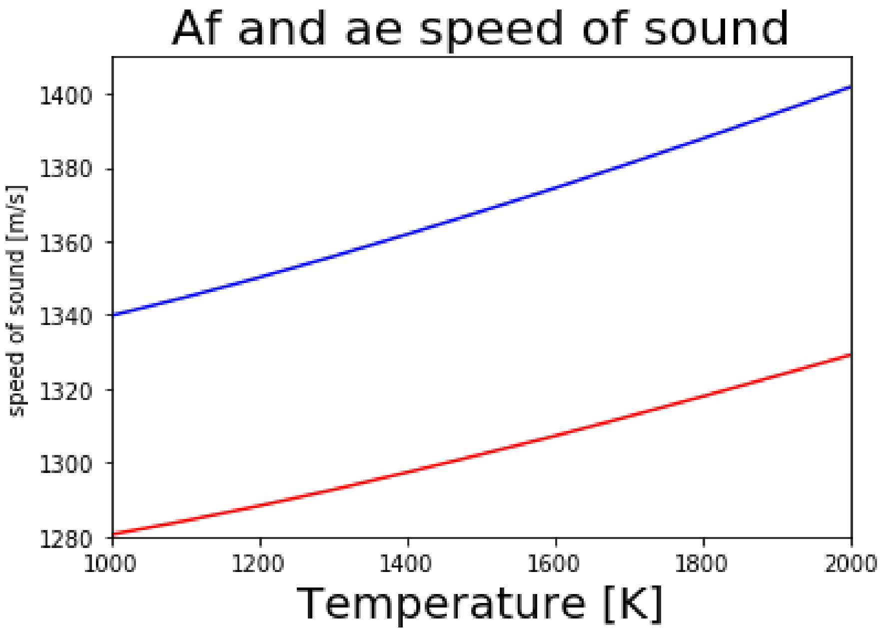

Figure 6: Influence of initial temperature on equilibrium sound speed (red line) and frozen sound speed (blue line).

Figures 2 - 6 show changes in Chapman-Jouguet detonation speed with increasing initial temperature.
The speed of detonation is decreasing a little.
The final temperature decreases to 3650K for initial temperature equals 1300K. Above this value, the final temperature starts increasing.
The final pressure is decreasing. The pressure is connected with a huge amount of energy. When energy is going out, the pressure is decreasing.
There is also noticed decreasing density of mixture for increasing initial temperature.
Speed sounds has greater values for greater values of initial temperature.

3.2 Results for $T = 1000K$, $\phi = 1$ and different initial pressure.

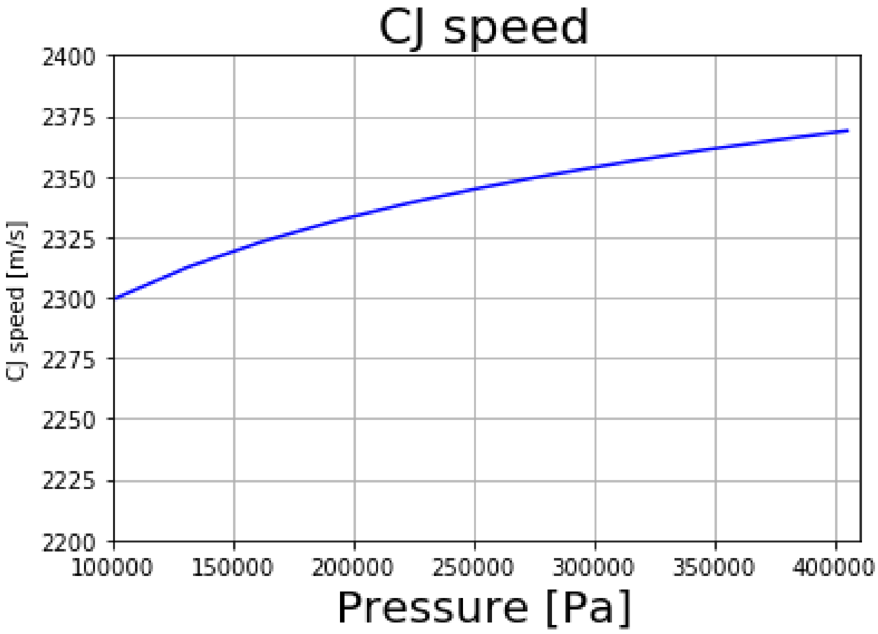

Figure 7: Influence of initial pressure on C-J detonation speed.

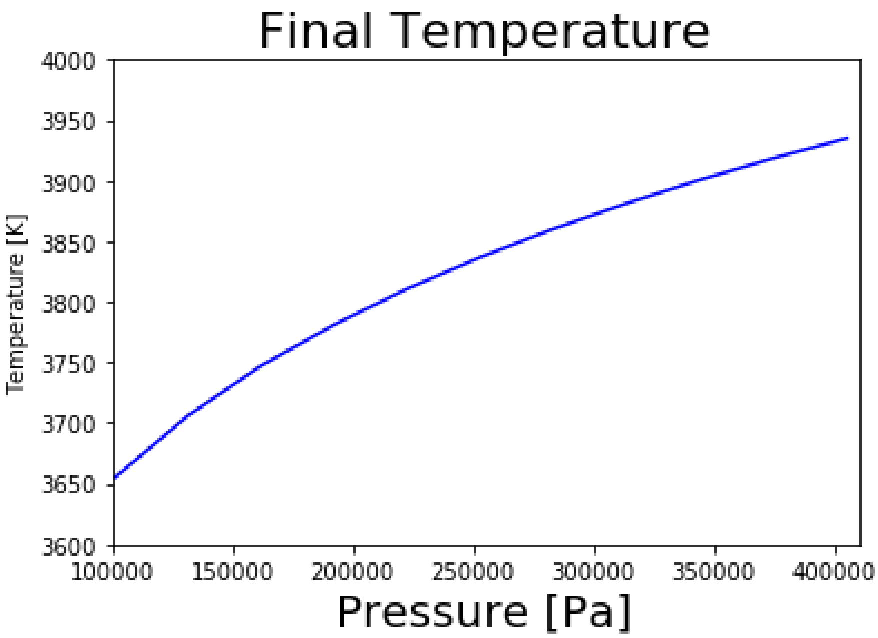

Figure 8: Influence of initial pressure on detonation temperature.

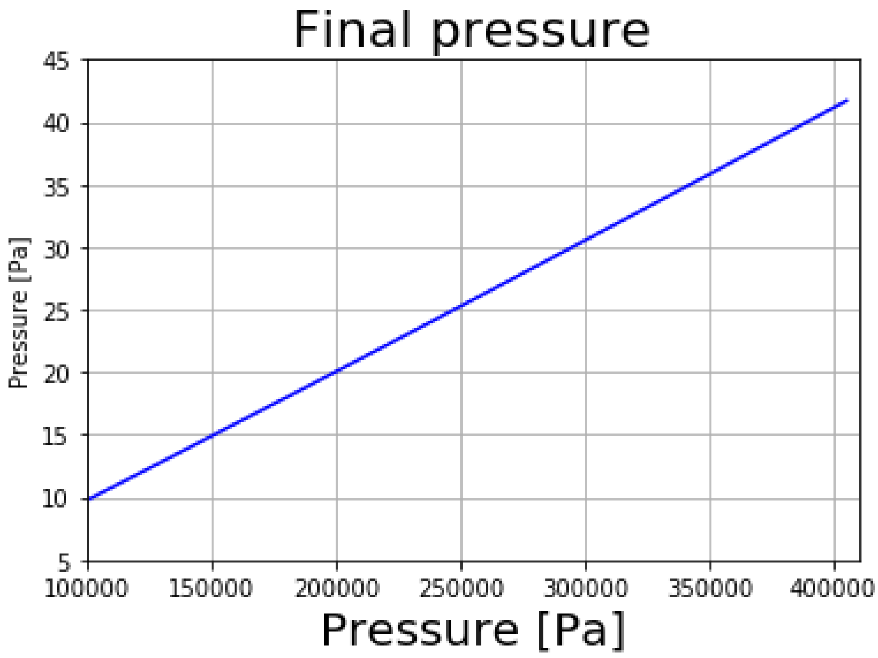

Figure 9: Influence of initial temperature on detonation pressure.

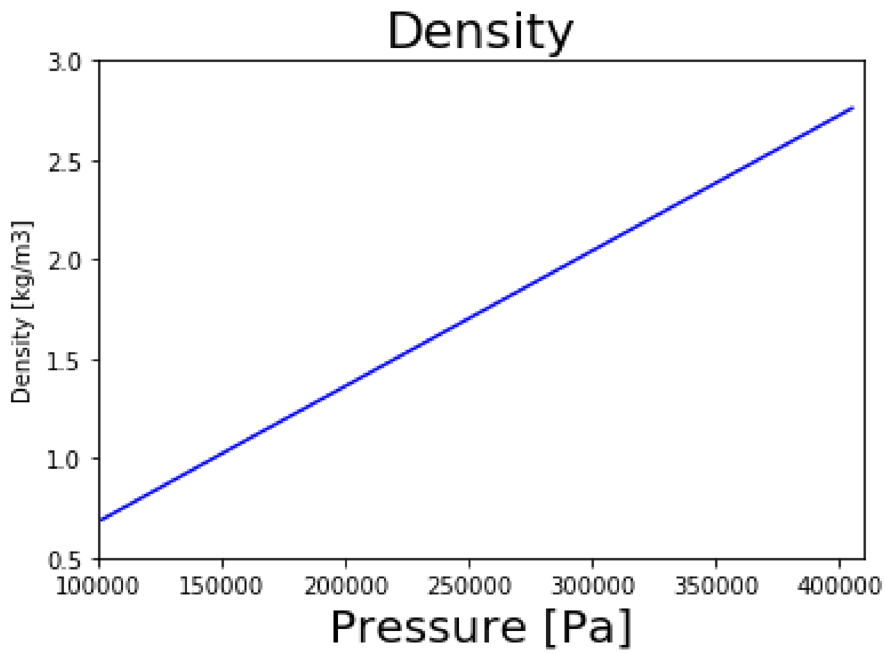

Figure 10: Influence of initial pressure on detonation density.

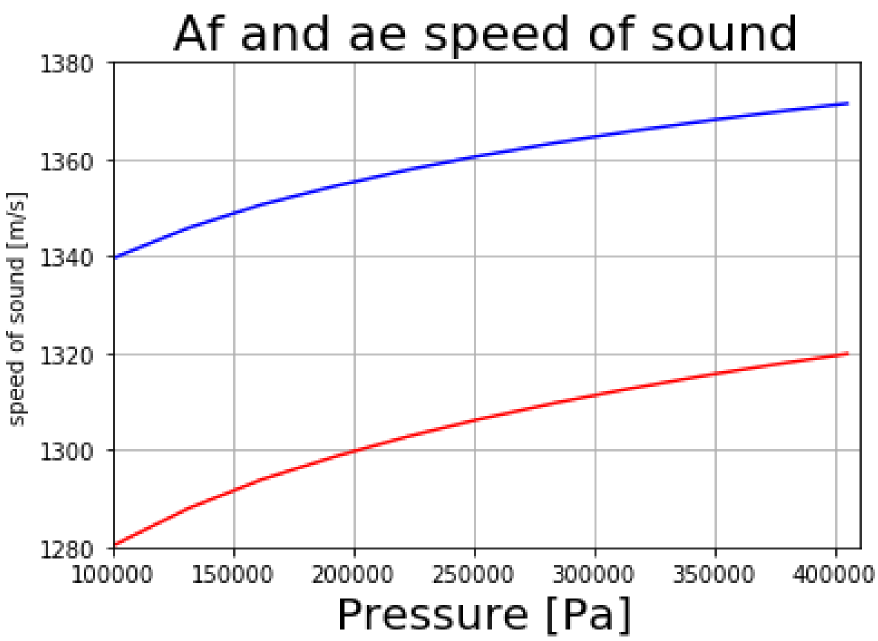

Figure 11: Influence of initial pressure on equilibrium sound speed (red line) and frozen sound speed (blue line).

Figures 7 - 11 show changes in Chapman-Jouguet detonation speed with increasing initial pressure. All of the calculating parameters (speed of detonation, final temperature, final pressure, density and speed of sound) are increasing.

3.3 Results for $T = 1000K$, $P = 1013,25hPa$ and different equivalence ratio values (ϕ).

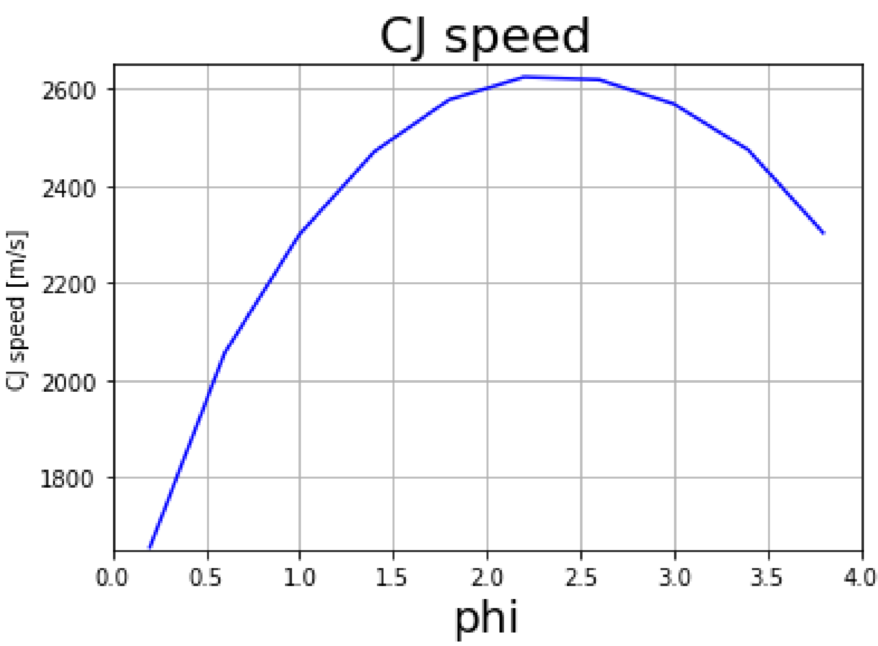

Figure 12: Influence of equivalence ratio on C-J detonation speed.

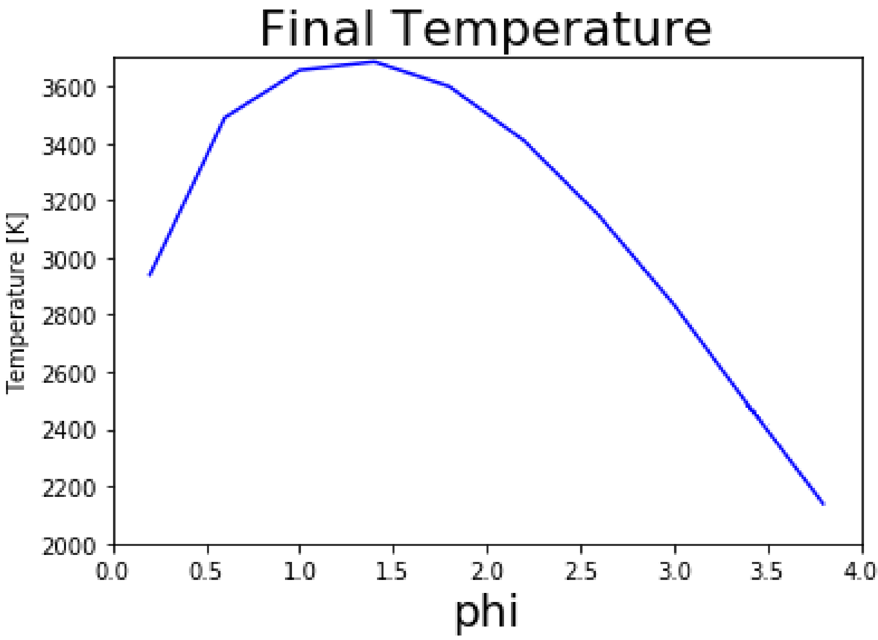

Figure 13: Influence of equivalence ratio on detonation temperature.

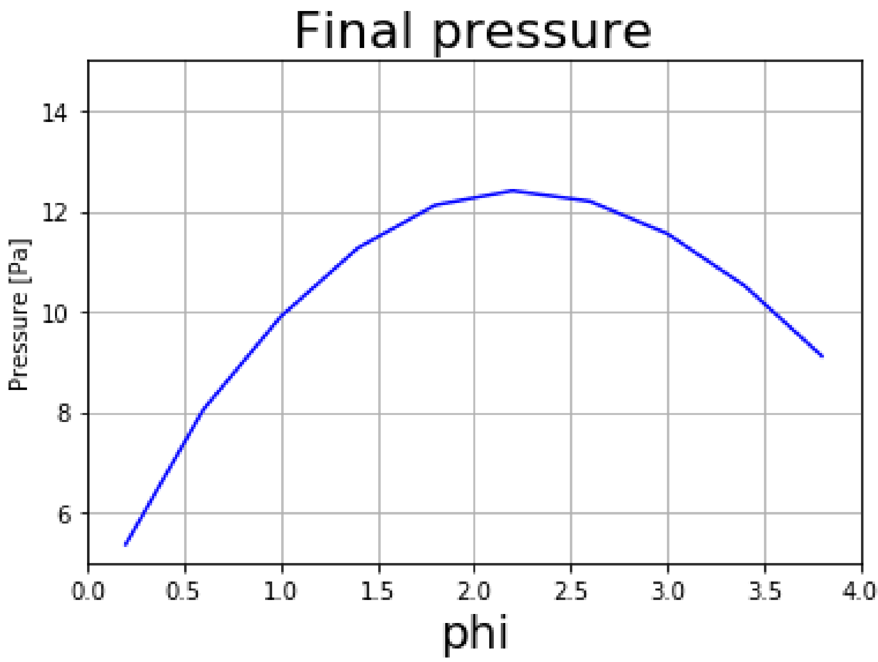

Figure 14: Influence of equivalence ratio on detonation pressure.

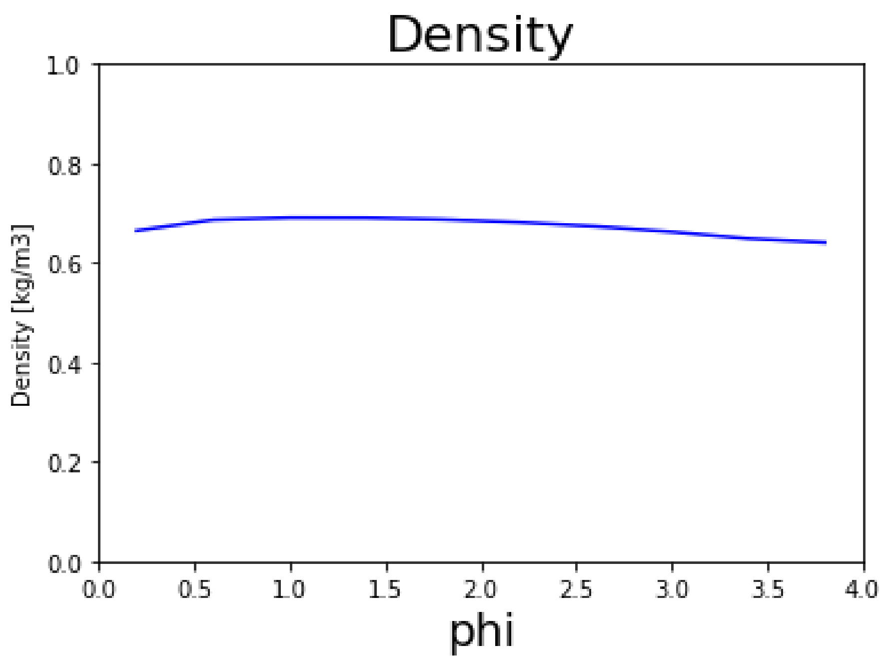

Figure 15: Influence of equivalence ratio on detonation density.

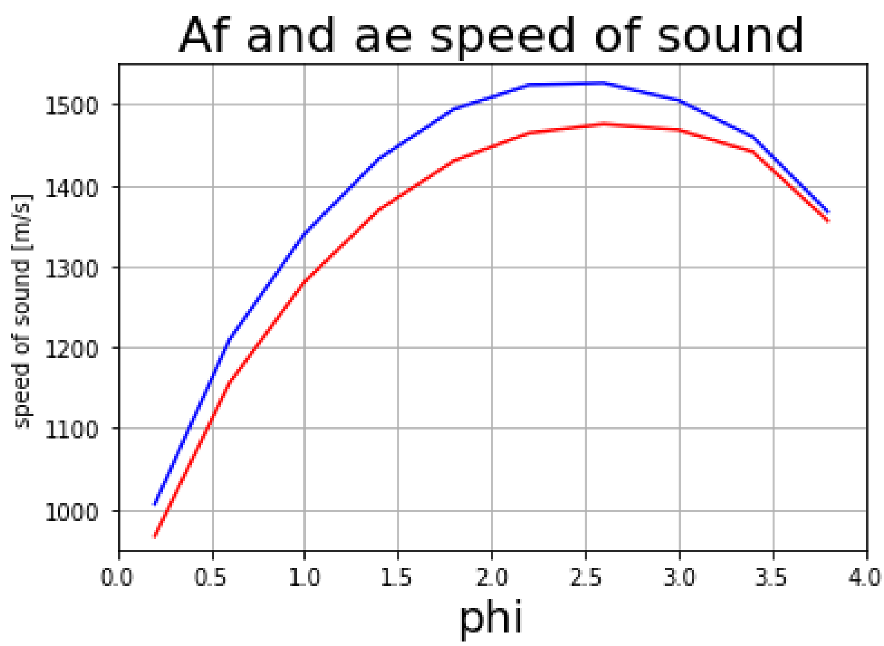

Figure 16: Influence of equivalence ratio on equilibrium sound speed (red line) and frozen sound speed (blue line).

Figures 7 - 11 show changes in Chapman-Jouguet detonation speed with increasing equivalence ratio. All of the calculating parameters except density have a parabolical character.
The greatest value of detonation speed is 2600 m/s for ϕ equals 2,25.
The greatest value of final temperature is 3700 K for ϕ equals 1,5.
The greatest value of final pressure is 12,3 atm for ϕ equals 2,25.
The density of final mixture is almost the same for different values of equivalence ratio.

The greatest values of sound speed are for ϕ equals 2,5.

4 Summary

The research gives information about the behavior of Chapman-Jouguet detonation with the parameters of temperature, pressure and ϕ. The data read from the plots are just approximation of the actual state. The more precise data are located in the .csv file (DS_SDT_EthaneOxygen.scv attached to the report). This file contains fully information about final temperature and autoignition timing for every investigated instantiation.

5 References

1. $CANTERA\_HandsOn.pdf$

2. Prediction of Detonation Pressure and Velocity of Explosives with Micrometer Aluminum Powders
   `https://www.mech.kth.se/courses/5C1219/Hand_out_PDF/SG2219_NT_Lecture`