Parameters of methane detonation using SD-Toolbox in Cantera

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Contents

1 Introduction

The purpose of the project was to evaluate the relation of initial parameters such as pressure and temperature to parameters after detonation. A mixture of methane and air were used in calculations. Calculations were performed using SDToolbox under Cantera.

2 Literature

According to [4]: "Cantera is a suite of object-oriented software tools for problems involving chemical kinetics, thermodynamics, and/or transport processes. Cantera is currently used for applications including combustion, detonations, electrochemical energy conversion and storage, fuel cells, batteries, aqueous electrolyte solutions, plasmas, and thin film deposition.". SDToolbox is an extension to Cantera which provides tools to solve shock and detonation problems.

3 Mathematical model

The stoichiometric reaction of complete combustion of methane in oxygen is as follows

$$2CH_4 + 4O_2 \rightarrow 4H_2O + 2CO_2$$

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

$$P_2 = P_1 + \rho_1 w_1^2 (1 - \frac{\rho_1}{\rho_2})$$

$$h_2 = h_1 + \frac{1}{2} w_1^2 (1 - (\frac{\rho_1}{\rho_2})^2)$$

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

$$P_2 = P_1 - \rho_1^2 w_1^2 (v_2 - v_1)$$

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 temperature after detonation.

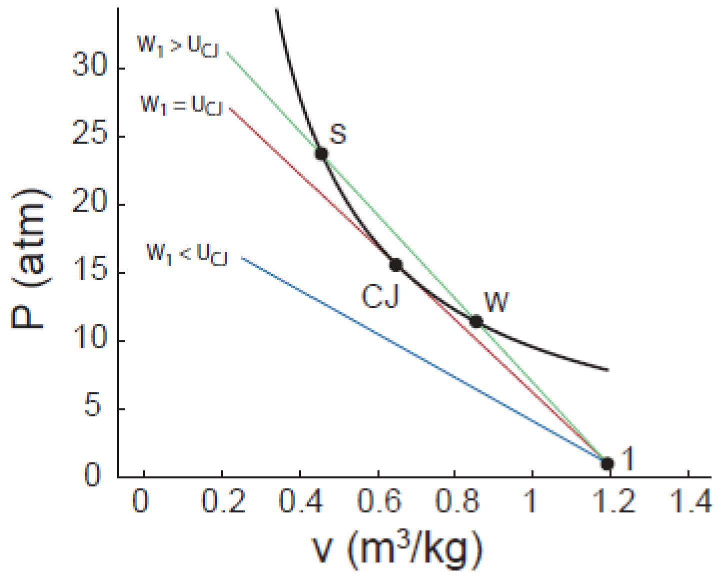

Figure 1: Rayleigh and Hugoniot lines

4 Code description

Gri30 mechanism was used for calculations.

Firstly, it was necessary to evaluate methane concentration for calculations. A value for which the value of post-detonation pressure was the highest was choosen. It happened to be around 10.65% of methane in air. Initial parameters for this step were:

- P0 = 1 atm
- T0 = 300 K

Then, for choosen concentration main calculations were performed. These included evaluating pressure, temperature and Chapman - Jouguet velocity. The results are shown in Results section.

Calculations were done using SDToolbox function CJspeed.

5 Results

Figure 2 shows result from calculation of pressure for various methane in air concentrations. The highest pressure value was for 10.65% of methane.

Figures 3 and 4 show changes in Chapman-Jouguet speed with increasing initial pressure and temperature. The speed also increases.

As can be seen from figures 5 and 6 the dependency of detonation parameters and initial parameters is linear. Calculations performed up to 50 atm of initial pressure didn't show any change. The character was always linear.

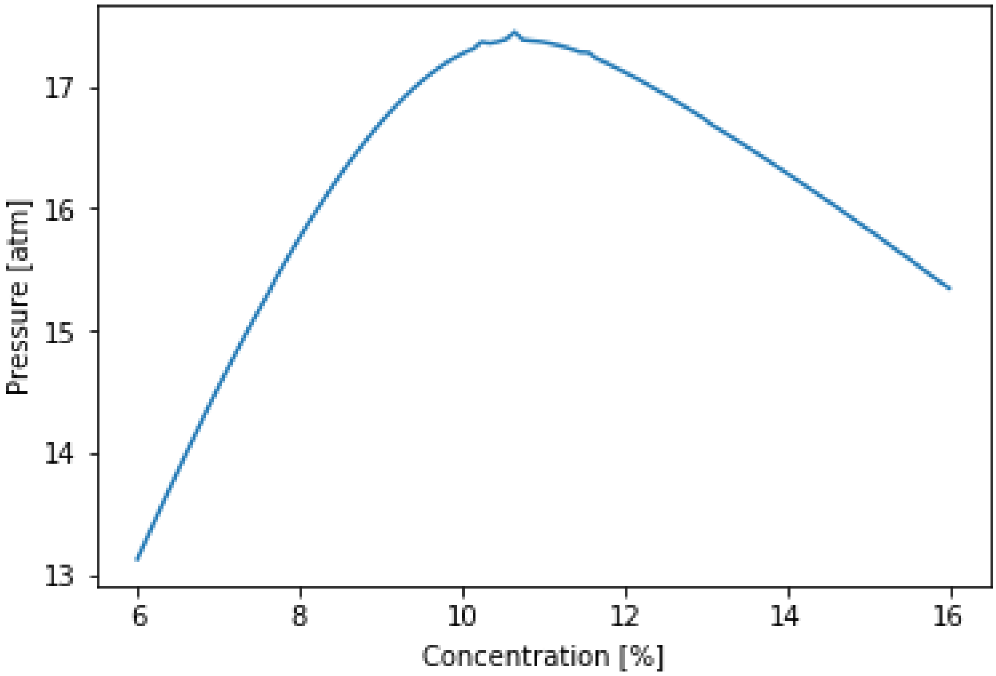

Figure 2: Detonation pressure for various concentration values

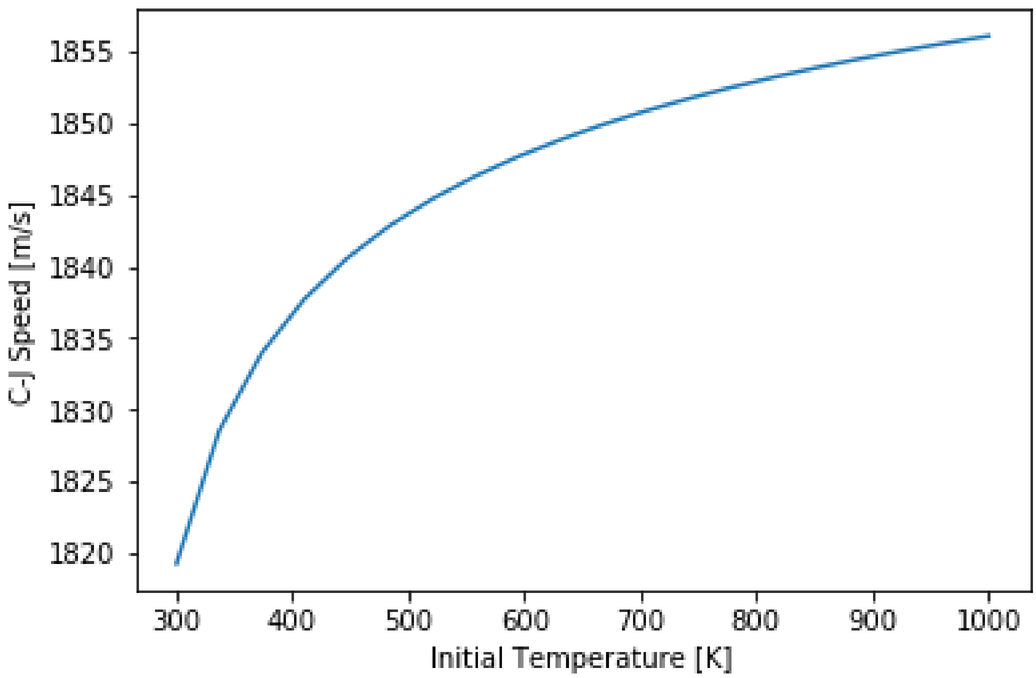

Figure 3: Chapman-Jouguet detonation speed for various initial temperature values

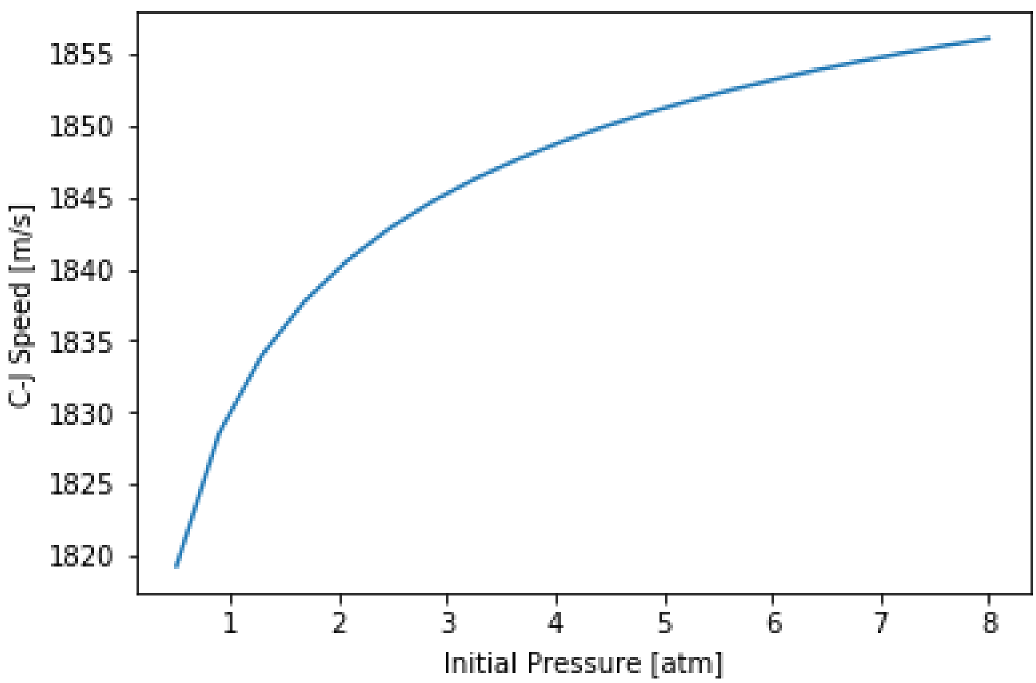

Figure 4: Chapman-Jouguet detonation speed for various initial pressure values

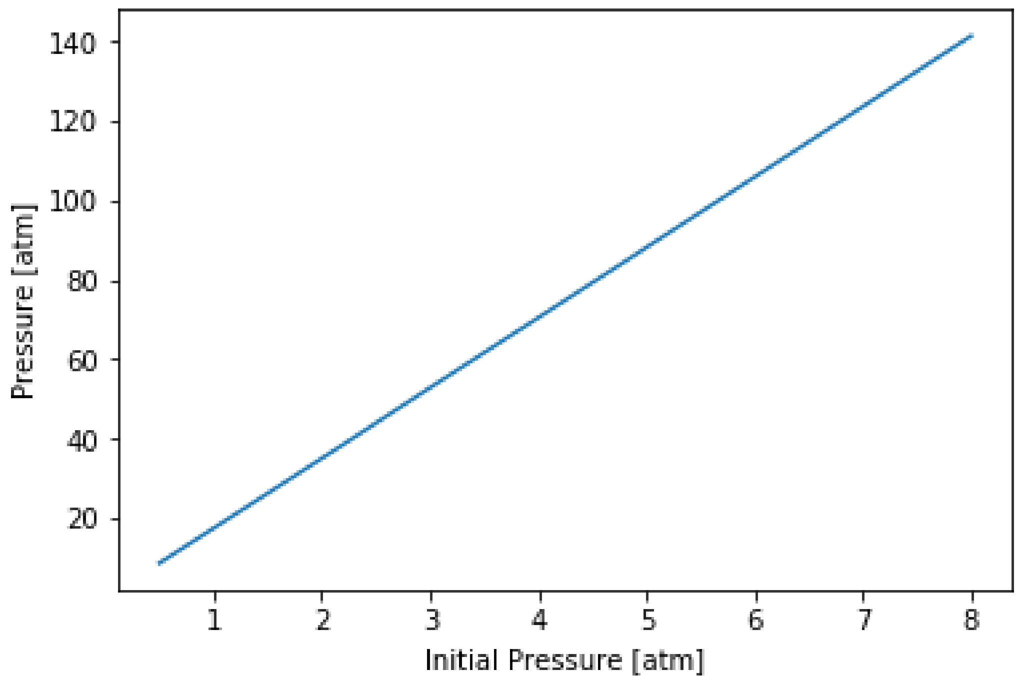

Figure 5: Detonation pressure for various values of initial pressure

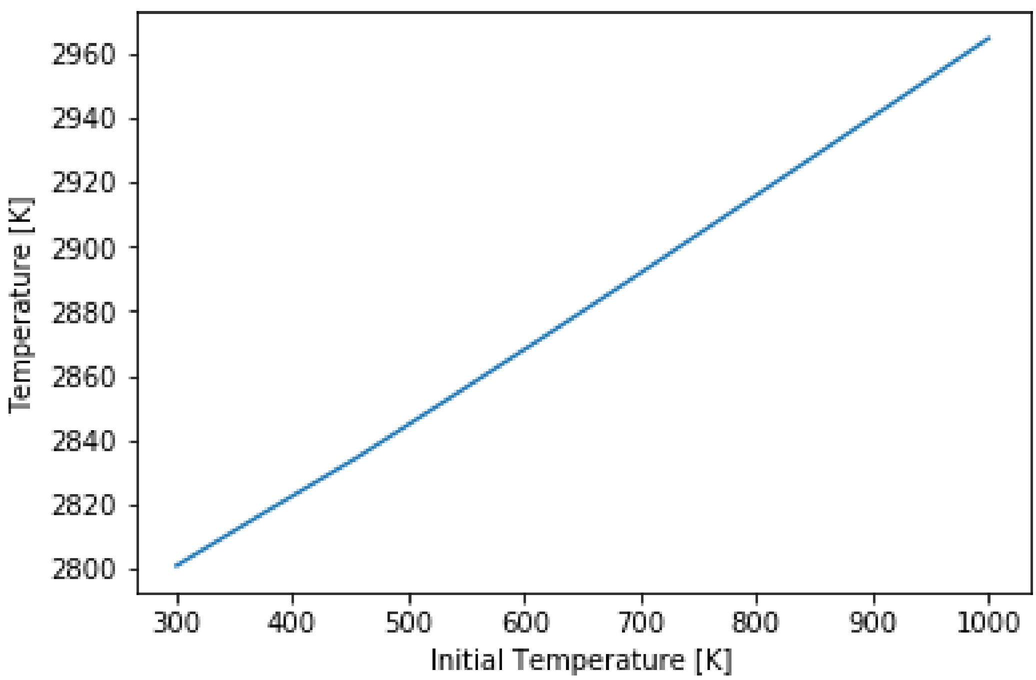

Figure 6: Detonation temperature for various values of initial temperature

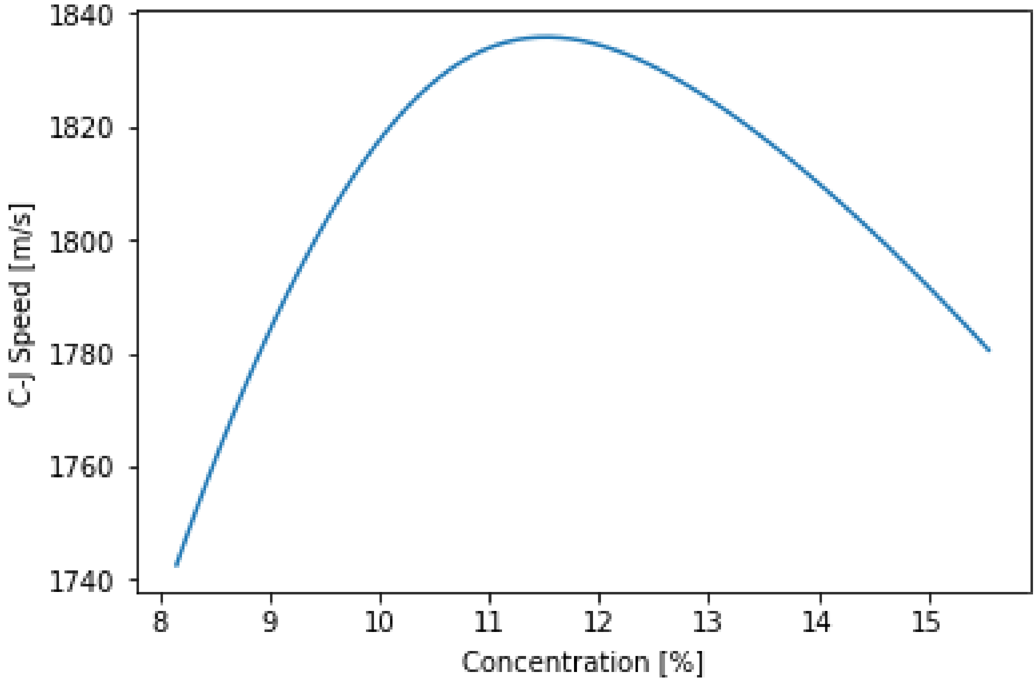

Figure 7: Detonation speed for various fuel concentration values

6 Summary

Detonation pressure and temperature are close to be a linear function of initial parameters. The highest values of parameters are to be found near 11% of fuel in air concentration.

References

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