PARAMETERS OF METHANE-OXYGEN DETONATION

Computational methods of combustion

PAWEL WALKUSKI

September 8, 2017

Faculty of Power and Aeronautical Engineering
Warsaw University of Technology
Computational methods in combustion

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 oxygen were used in calculations.

2 METHODS

SDToolbox under Cantera was used for calculations.

2.1 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 above, we can conclude that ratio by volume for combustion of methane in oxygen is $\frac{1}{2}$. That gives us methane concentration for stoichometric conditions, which is 50%.

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.

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

2.2 Code description

Calculating mixture composition for various methane concentration values is according to equation:

$$x = \frac{n_{CH_4}}{n_{CH_4} + n_{O_2}}$$

where x - methane concentration, n_{CH_4} - number of moles of methane, n_{O_2} - number of moles of oxygen. For simplicity, n_{O_2} was set to 1.

Code uses functions CJspeed and PostShock_eq from SDToolbox to calculate post-shock state of gas.

3 RESULTS

Figures 1, 2, 3 show influence of various methene in oxygen concentration for detonation parameters. Highest values occur for near stoichometric concentration values. Calculations were performed for $T = 300K$ and $P = 1bar$.

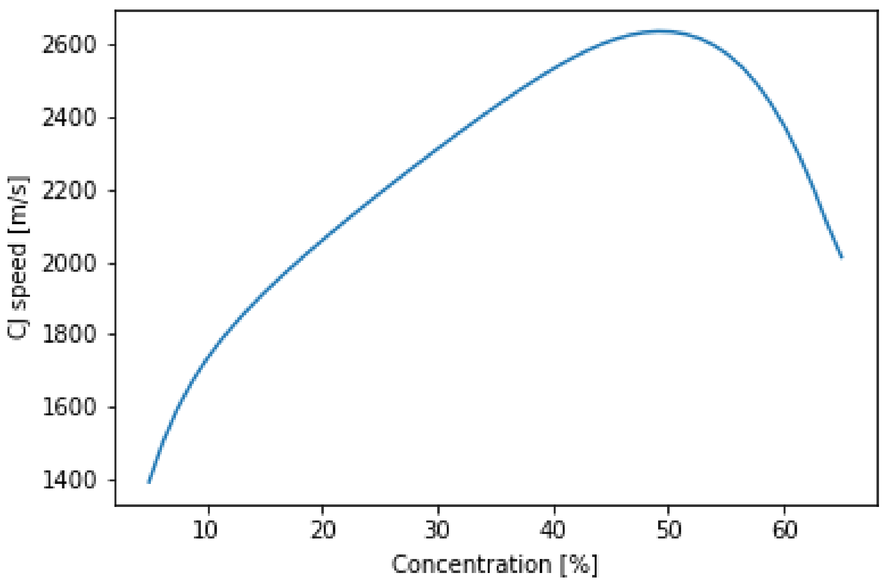

Figure 1: CJ speed for varying methane concentration

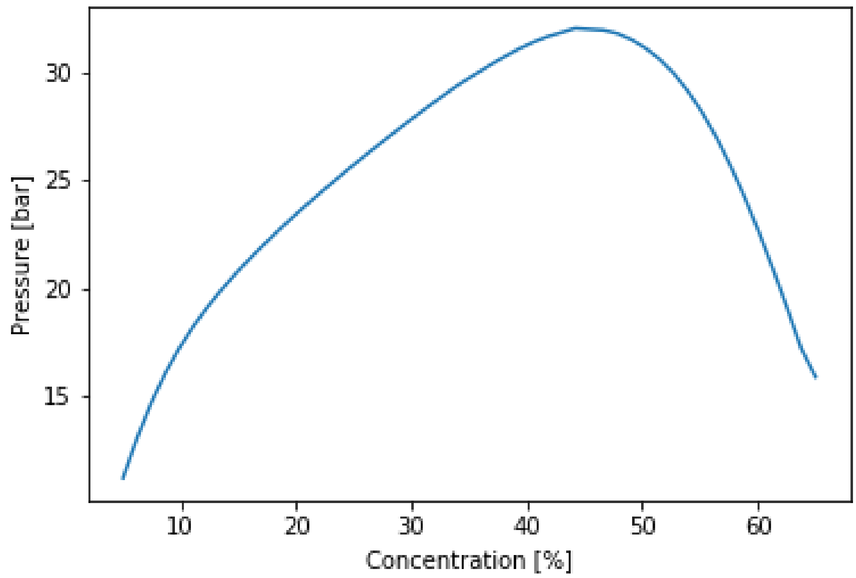

Figure 2: Post shock pressure for varying methane concentration

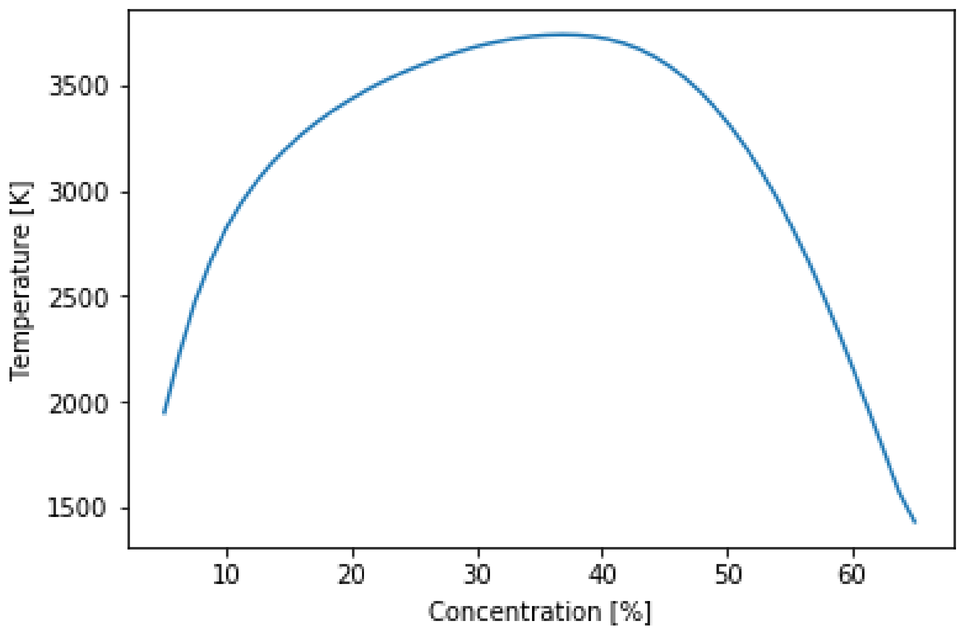

Figure 3: Post shock temperature for varying methane concentration

Figures 4, 5, 6, 7 show influence of initial conditions for post-shock parameters.

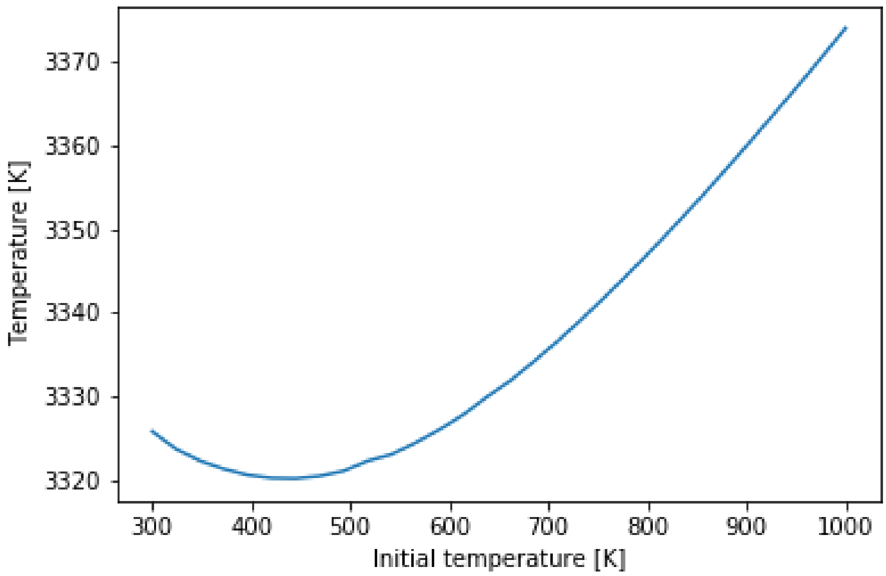

Figure 4: Post shock temperature for various initial temperature values

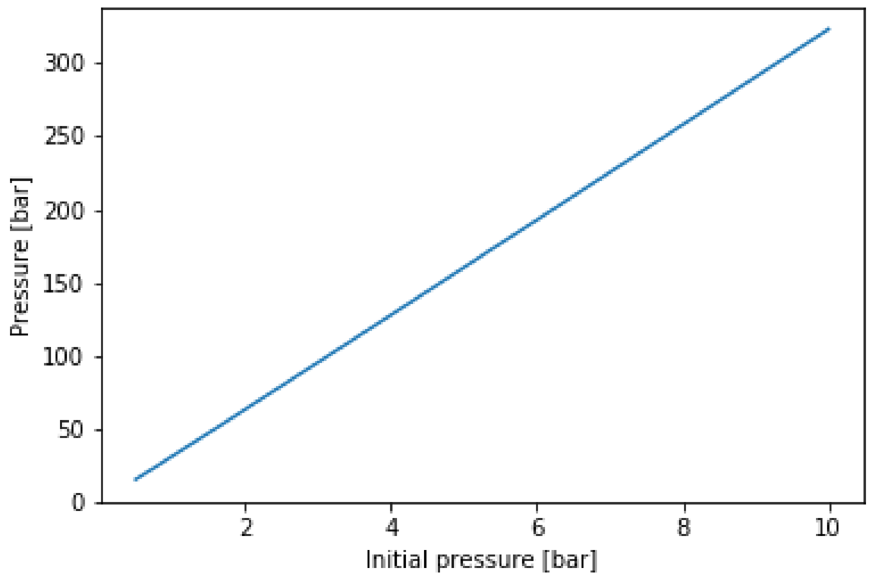

Figure 5: Post shock temperature for various initial temperature values

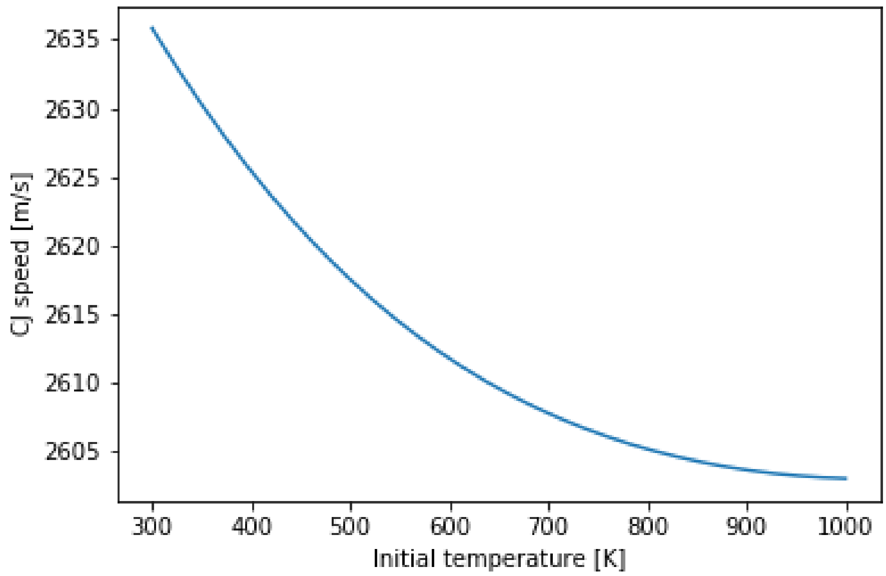

Figure 6: CJ speed for various initial temperature values

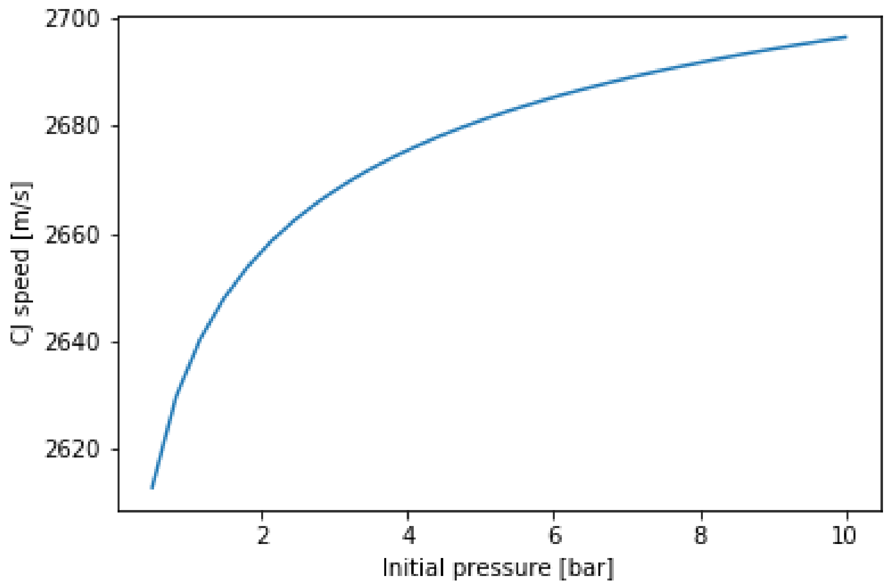

Figure 7: CJ speed for various initial pressure values

4 SUMMARY

Detonation parameters for methane-oxygen mixture proved to be highly dependent on fuel concentration and initial conditions. Highest values, as expected, occur for concentration for which the stoichometric ratio is close to one.

REFERENCES

[1] Cantera http://www.cantera.org/docs/sphinx/html/index.html

[2] SDToolbox http://shepherd.caltech.edu/EDL/public/cantera/html/SD_Toolbox/