Computational methods of combustion

Detonation of methane – oxygen mixture for different initial temperature, pressure and concentration

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1. Introduction

The purpose of this project is to conduct simulation of Chapman-Jouguet detonation for various methane oxygen mixtures and show the relation between C-J detonation speed of the said mixture and initial temperature as well as initial pressure and concentration. The simulations were performed using Cantera and SDToolbox packages in Python.

2. Mathematical model

The stoichiometric reaction of complete combustion is shown below:

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

The methane concentration for stoichiometric conditions is 50%.
Jump conditions for a detonation can be expressed by the following formula using conservation equations:

$$P_2 = P_1 + \rho\omega_1^2 \, (1 + \rho_1/\rho_2)$$

$$h_2 = h_1 + 0.5\omega_1^2 \, (1 + (\rho_1/\rho_2)^2)$$

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

$$P_2 = P_1 - \rho_1^2\omega_1^2(\nu_2 - \nu_1)$$

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

$$h_2 - h_1 = 0.5(P_2 - P_1)(\nu_2 + \nu_1)$$

The minimum wave speed occurs Rayleigh line is tangent with Hugoniot. The tangent point is referred to as C-J state.

Calculations were performed for temperature and pressure range of 300K to 1000K and 0.5atm to 10atm respectively as well as for different mixture concentration.

3. Results

Figure 1 shows C-J speed for φ = 50 % and p = 1 atm.

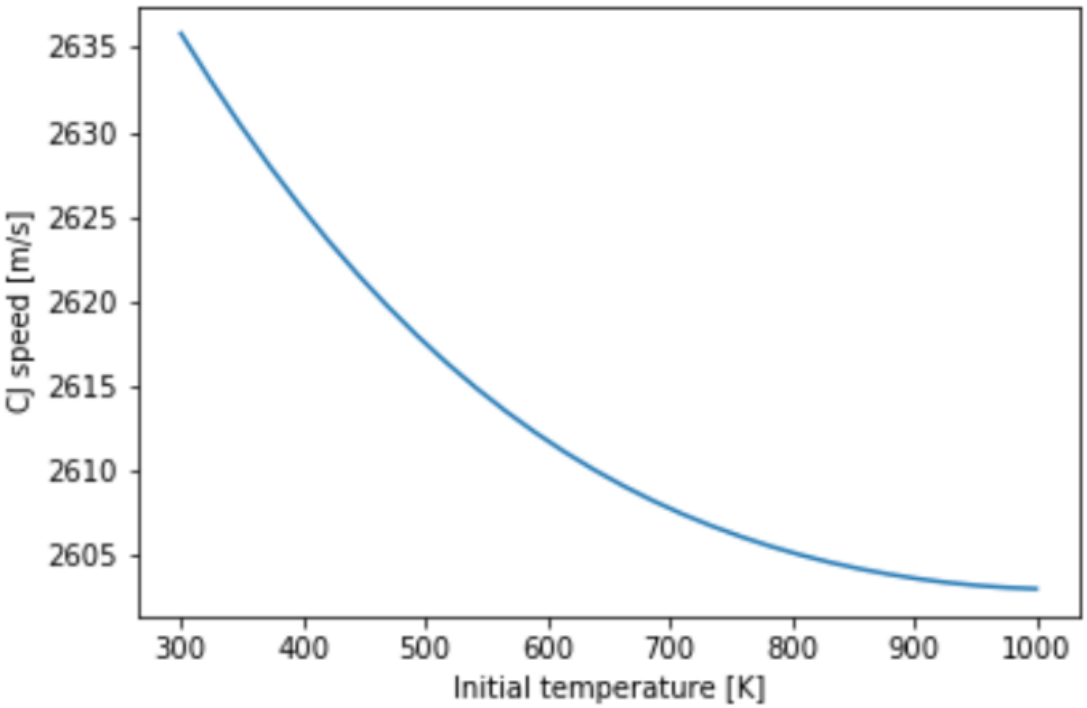

Figure 1. C-J speed dependence on various initial temperature

Figure 2 shows C-J speed for T = 500 K, φ = 50 %.

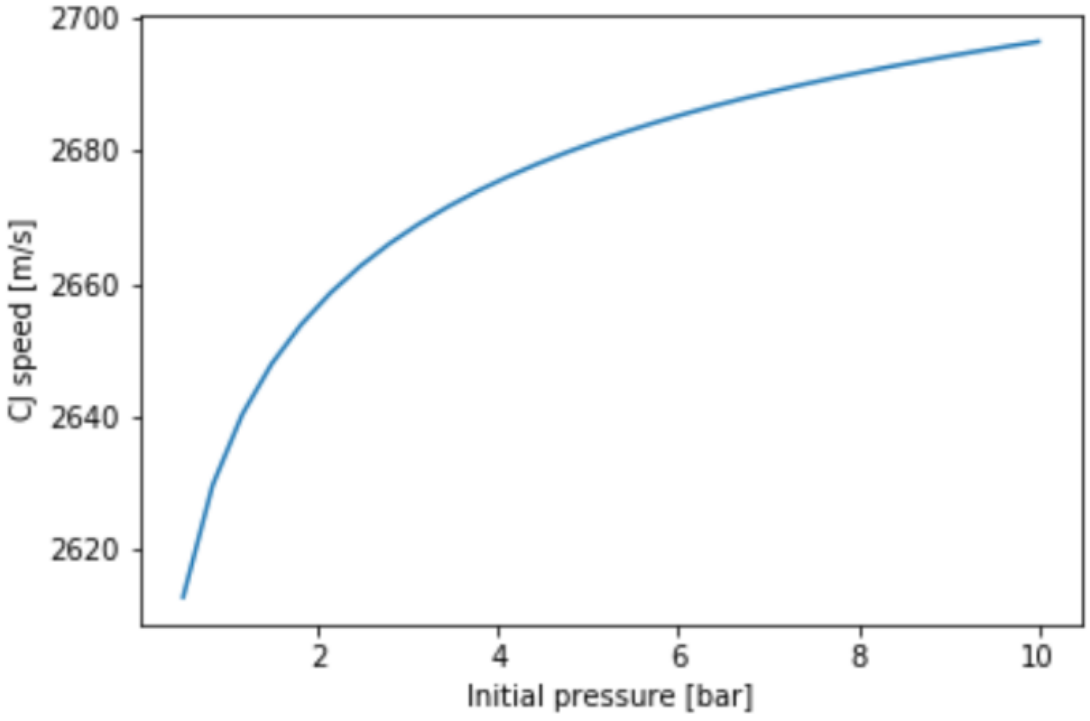

Figure 2. C-J speed dependence on various initial pressure

Figure 3 shows C-J speed for T = 500 K and p = 1 atm.

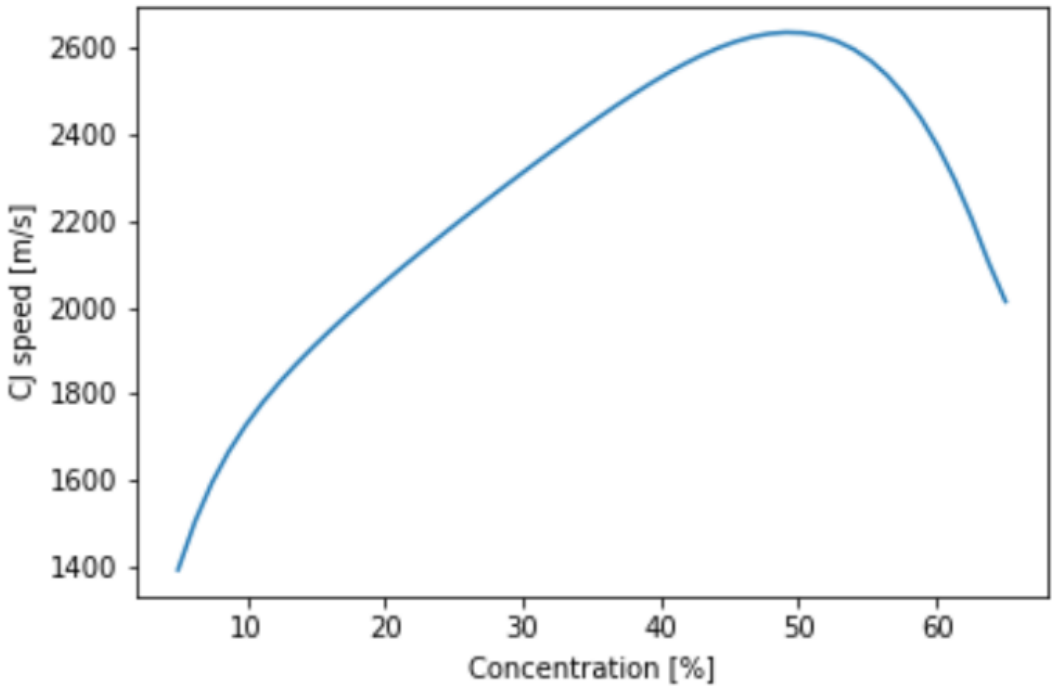

Figure 3. C-J speed dependence on mixture concentration

4. Conclusion.

a) C-J speed decreases for higher value of initial temperature.
b) C-J speed increases for higher value of initial pressure.
c) C-J speed is much influenced by the mixture concentration. The highest speed can be observed for concentration with stoichiometric ratio $\varphi \sim 1$.

5. References.

http://shepherd.caltech.edu/EDL/public/cantera/html/SD_Toolbox/

http://cantera.org/docs/sphinx/html