Metody Komputerowe w Spalaniu - Cantera (SDToolbox) Project: Detonation Velocity of Hydrogen

Krzysztof Górka

August 2018

1 Introduction

In this project i am taking into consideration the detonation of hydrogen in air. I am going to calculate CJ Detonation speed for different initial conditions using Cantera and SDToolbox which is a collection of numerical routines that enables the solutions to of standard problems for gas-phase explosions using realistic thermochemistry and detailed chemical kinetics

2 Literature

1. http://shepherd.caltech.edu/EDL/public/cantera/html/SDToolbox/
2. https://www.mech.kth.se/
3. http://seitzman.gatech.edu/classes/ae3450/rayleighflowtwo.pdf
4. M.Gieras "Spalanie - Wybrane zagadnienia w zadaniach"

3 Description of model

The stechiometric reaction is given:
$2H2 + O2 + 3,76N2 \rightarrow 2H20 + 3,76N2$

Regarding to [2] jump conditions for detonations are:

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

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

The Rayleigh line ([3] a straight line connecting points corresponding to the initial and final states on a graph of pressure versus specific volume for a substance subjected to a shock wave) is:
$P_2 = P_1 - (\rho_1)^2(\omega_1)^2(v_2 - v_1)$

Hugoniot/shock adiabat equation (formula describing the thermodynamic process to which gas is subjected flowing through shock wave):
$h_2 - h_1 = \frac{(P_2-P_1)(v_1+v_2}{2}$

When Rayleigh line is tangent to Hugoniot adiabat we have the minimum wave speed. The point of tangency is reffered to as the CJ state - from the coordinates of this point we can collect information on the pressure and temperature after detonation.

4 Description of the results

In this project calculations were made using Gri30 mechanism

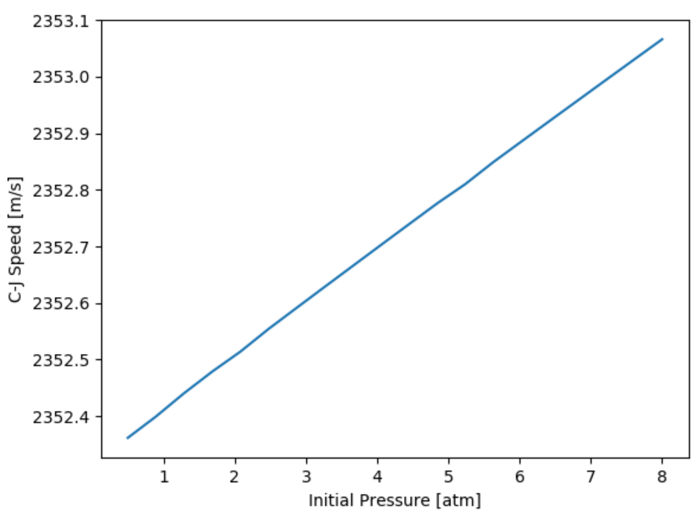

Figure 1: CJ-speed for different pressures

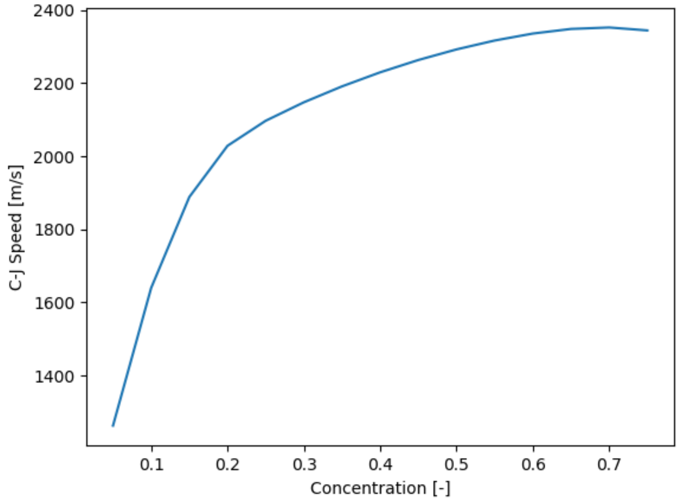

Figure 2: CJ-speed for different concentrations

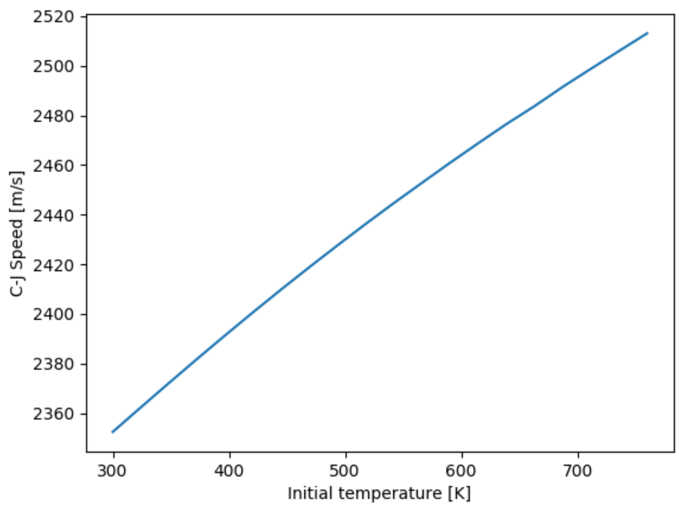

Figure 3: CJ-speed for different initial temperatures