Metody Komputerowe w Spalaniu - Cantera (SD-Toolbox) Project: Parameters of Methane Detonation

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1 Introduction

In this project am I taking into consideration the detonation of Methane in Air. I am going to calculate parameters of detonation (CJ detonation speed and post-detonation state) for different initial conditions using Cantera and SD-Toolbox - The Shock and Detonation Toolbox which is a collection of numerical routines that enables the solution 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/SD$_{T}$*oolbox*/
2. https://www.mech.kth.se/
3. https://encyclopedia2.thefreedictionary.com/Rayleigh+line
4. https://www.meil.pw.edu.pl

3 Description of the Model

I am starting with a stechiometric chemical reaction:

$CH_4 + 2O_2 + 7,52N_2 \longrightarrow CO_2 + 2H_2O + 7,52N_2$

Regarding to source [2] jump condtions for detonation are:

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

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

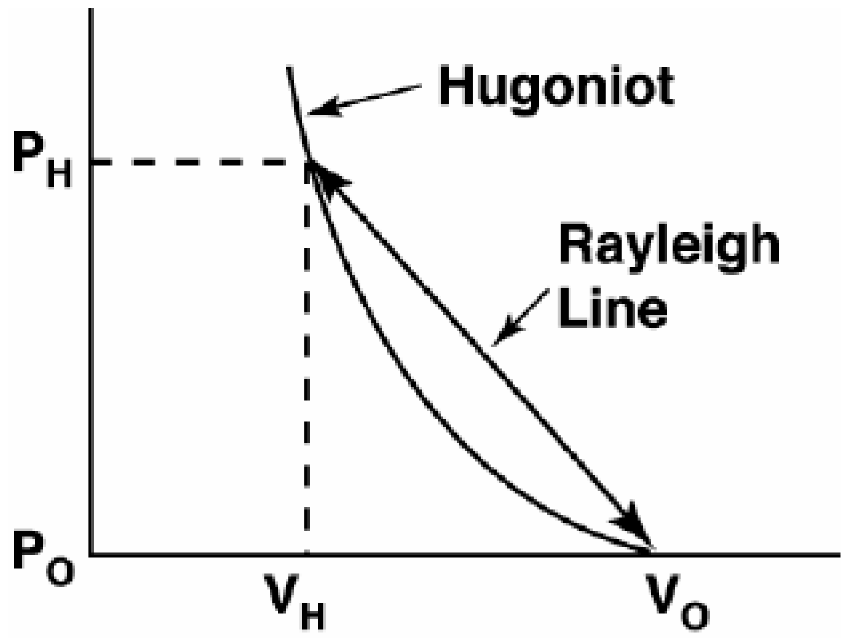
The Rayleigh line ([3] a straight line connecting points corresponding to the initial and final states on a graph of pressure versus specific volume for a substance subjected to a shock wave) is:

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

Hugoniot/shock adiabat equation ([4] formula describing the thermodynamic process to which gas is subjected flowing through shock wave):

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

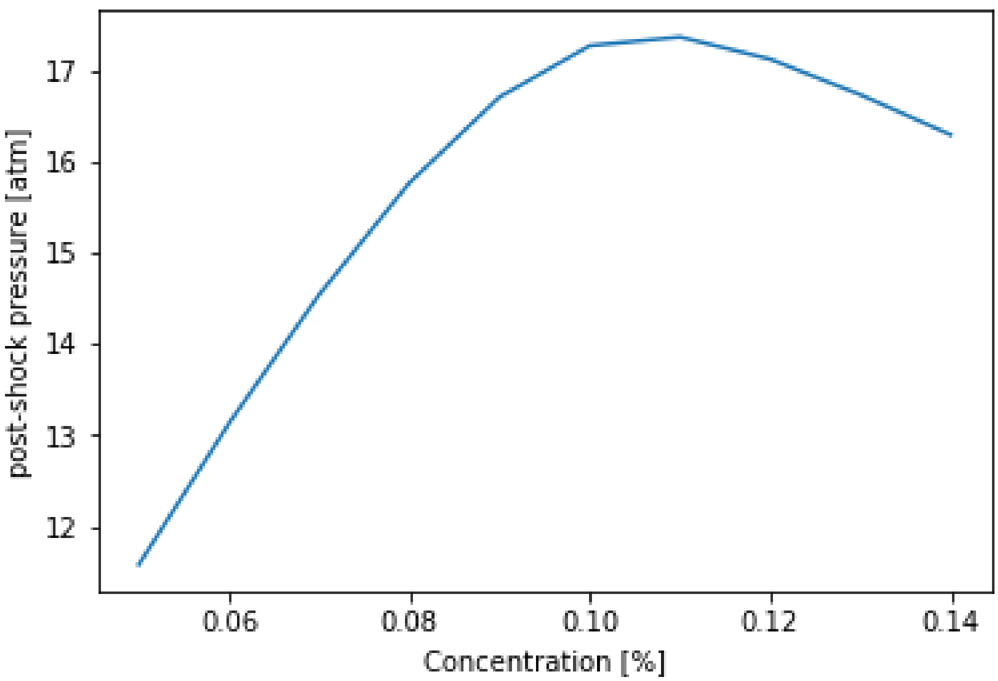
When Rayleigh line is tangent to Hugoniot adiabat we have the minimum wave speed. The point of tangency is reffered to as the CJ state - from the coordinates of this point we can collect information on the pressure and temperature after detonation.



4 Description of the Results

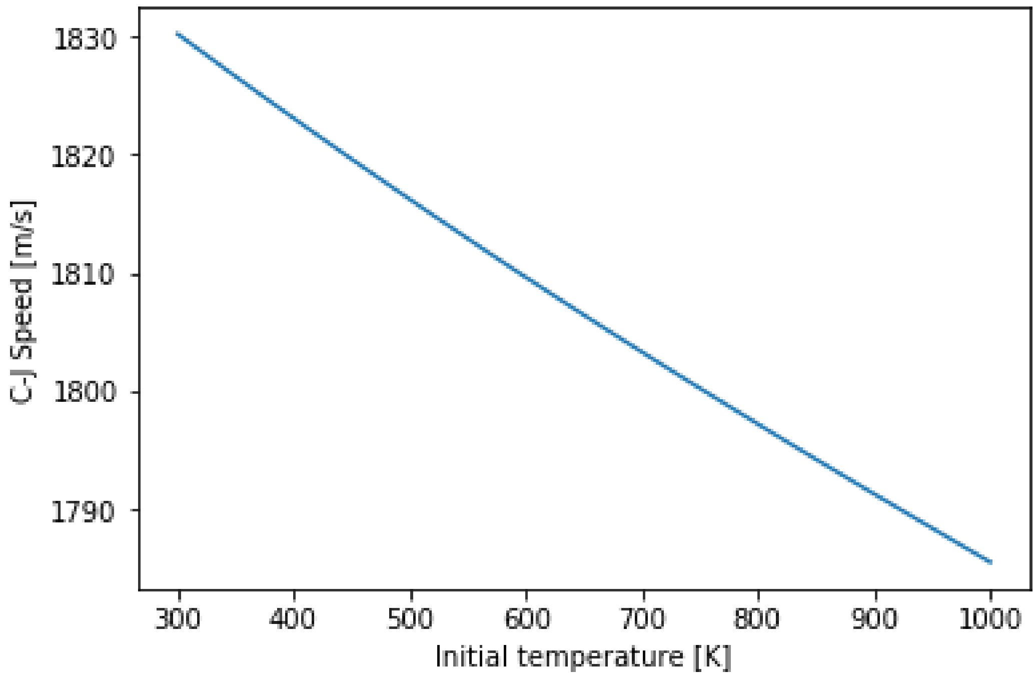
In this project I am doing calculations using Gri30 mechanism.

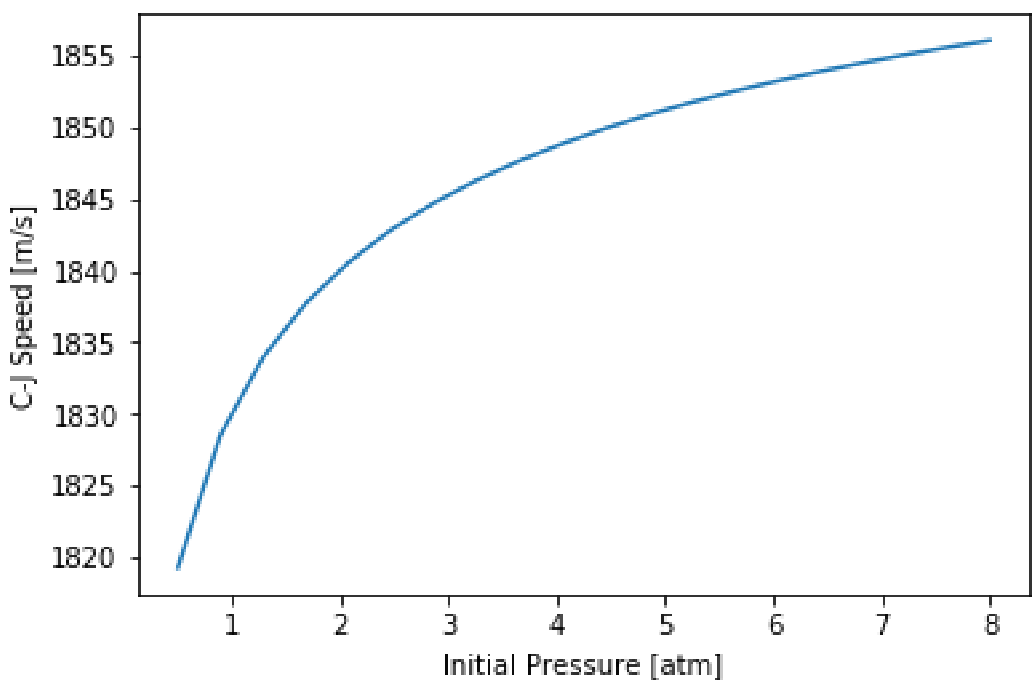
GRAPH 1:



Initial parameters for first plot are
$P_0 = 1atm$
$T_0 = 300K$
Max. pressure is reached for concentration of 10,65 percent of methane in air.

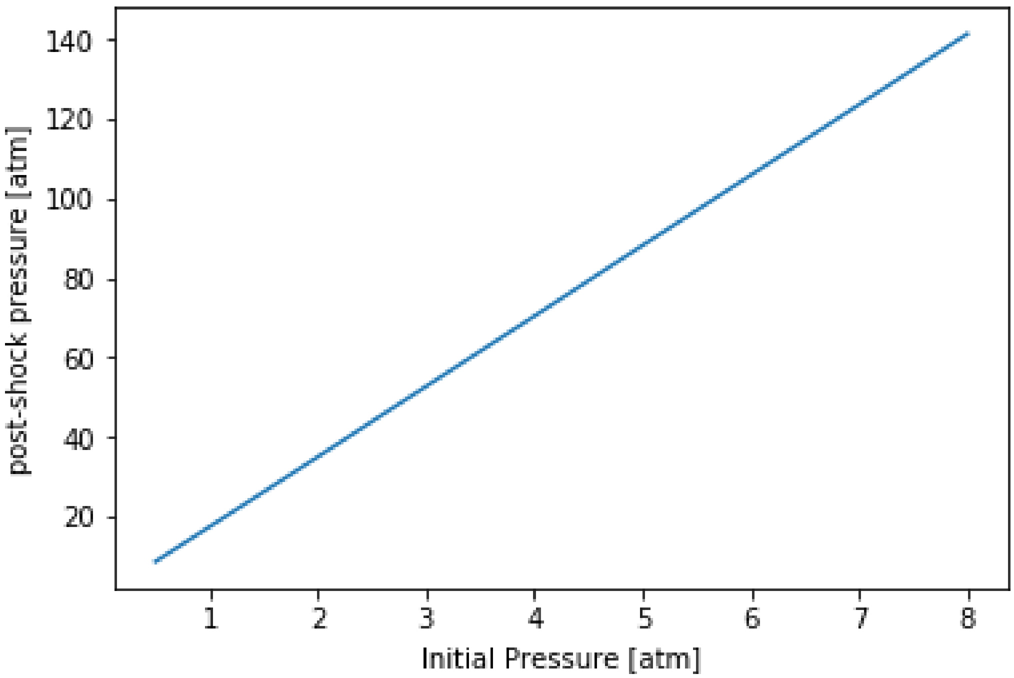
GRAPH 2,3:

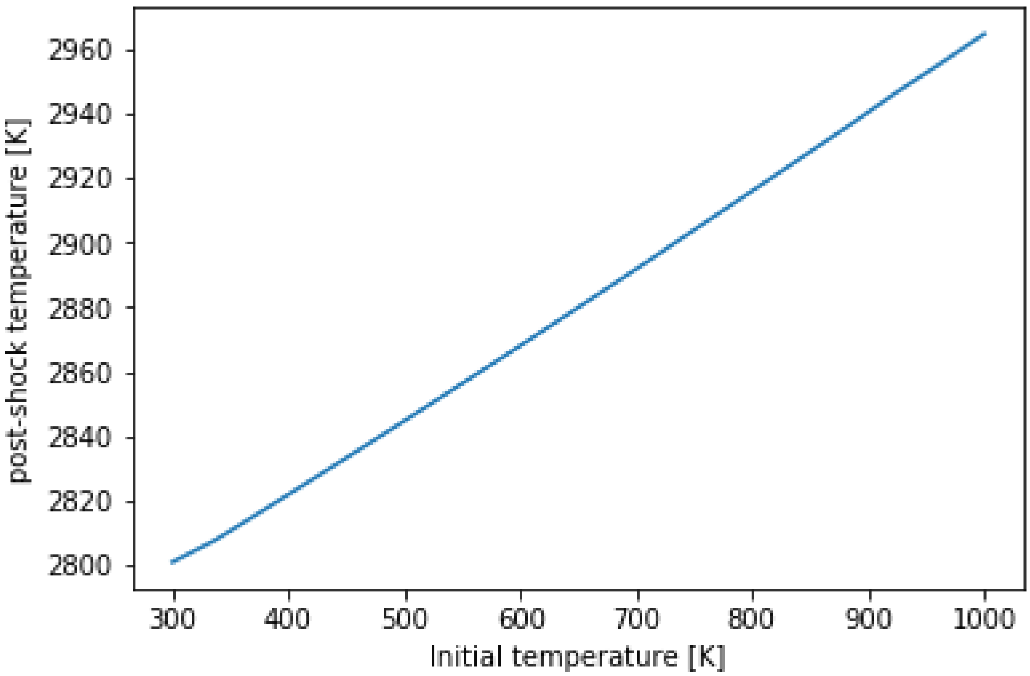




Both graphs are showing CJ speed - one for different initial temperatures and the other one for different initial pressures. In both cases CJ speed is the higher the higher initial parameter is.

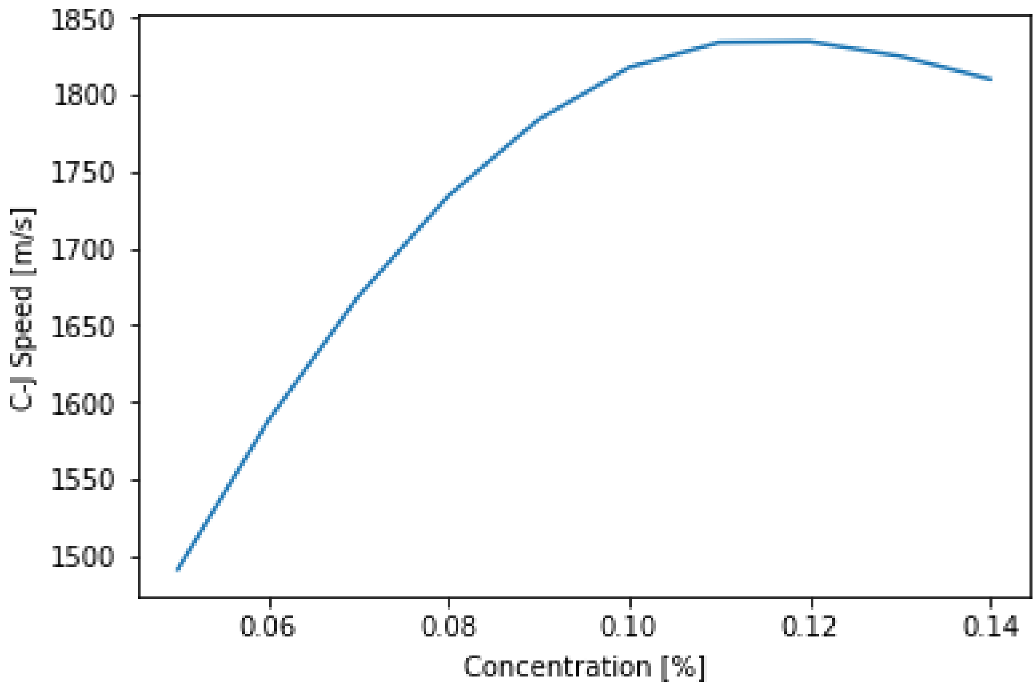
GRAPH 4,5:





Both functions of pressure/temperature from their initial parameters ale linear.

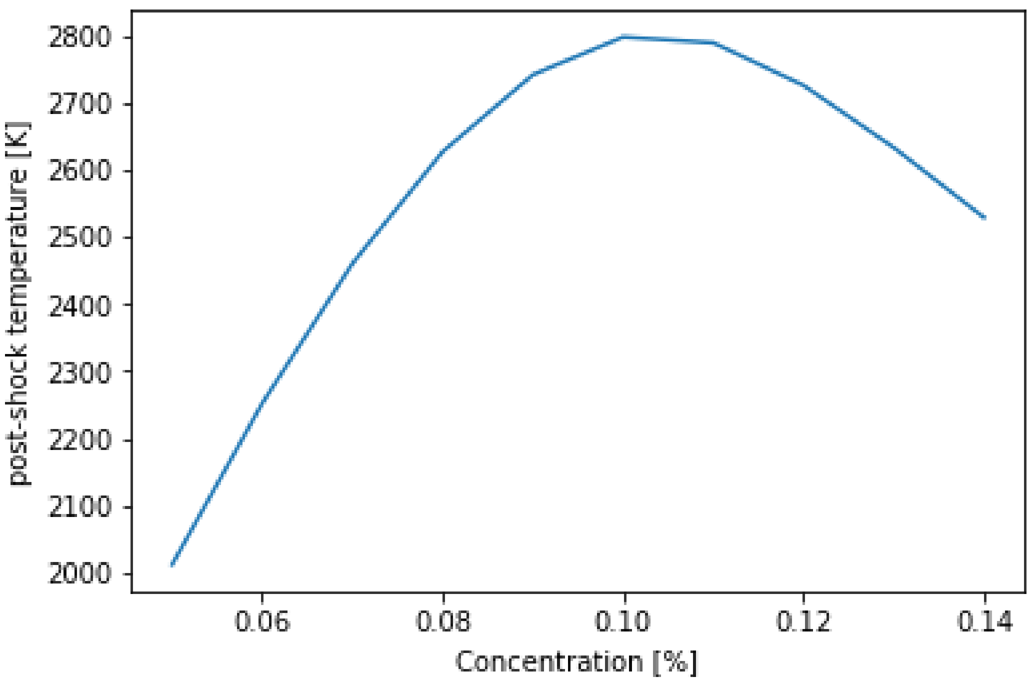
GRAPH 6:



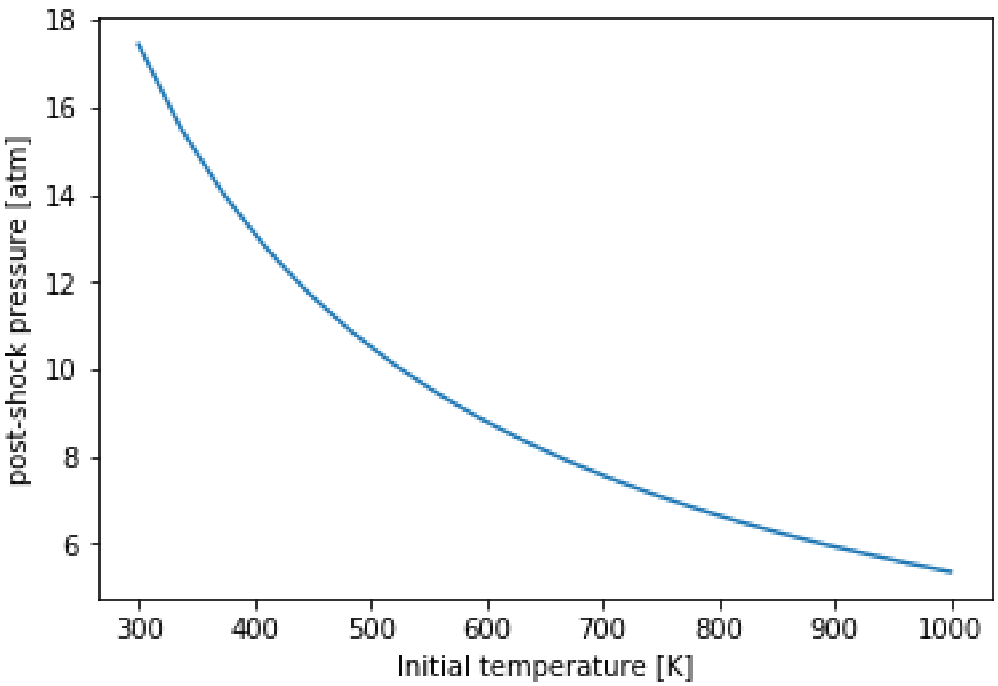
Next figure is CJ speed changing with concentration. The highest result is for concentration around 11 percent.

GRAPH 7 AND 8:

Last additional figures are Temperature changing with Concentration and Pressure changing with Initial Temperature:



2800
2700
2600
2500
2400
2300
2200
2100
2000
post-shock temperature [K]
0.06
0.08
0.10
0.12
0.14
Concentration [%]



18
16
14
12
10
8
6
post-shock pressure [atm]
300
400
500
600
700
800
900
1000
Initial temperature [K]