Detonation of propane - oxygen mixture

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Abstract

This project will be dedicated to simulated detonation of propane - oxygen mixture with different starting parameters, which are: temperature, pressure and equivalence ratio. The purpose is to calculate and analyze mentioned phenomenon parameters. The simulation was conducted using SDToolbox and Cantera libraries in python 2.7.

0.1 Definition of detonation

Detonation is a process of chemical transformation of an explosive that is accompanied by liberation of energy, which propagates through the substance as waves from one layer to another with supersonic speed. The chemical reaction is introduced by an intense shock wave, which forms the leading front of the detonation wave. Because of the sharp rise in temperature and pressure behind the front of the shock wave, the chemical transformation takes place extremely rapidly in the very narrow layer immediately adjacent to the wave front.

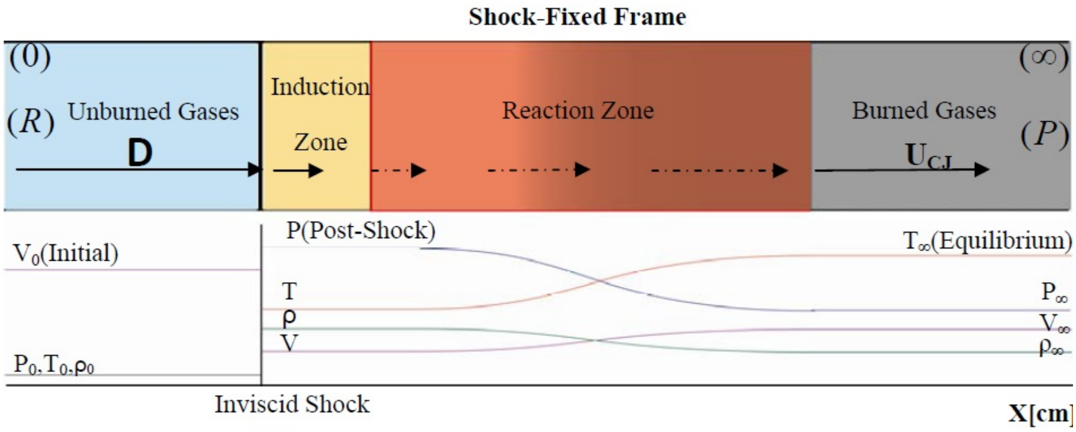

Figure 1.3. Schematic diagram of pressure, temperature, density, and velocity in Zel'dovich-von Neumann-Doering detonation

0.2 Mathematical model

SDToolbox is based on one-dimensional model of detonation, which was presented by Champan and Jouguet.
Below is being shown an equations of mass, momentum and energy, where:

ρ - density
u - speed of detonation wave
p - pressure
h - enthalpy

$$\rho_1 u_1 = \rho_2 u_2$$

$$p_1 + \rho_1 u_1^2 = p_2 + \rho_2 u_2^2$$

$$h_1 + \frac{1}{2} u_1^2 = h_2 + \frac{1}{2} u_2^2$$

Figure 1: Equations of preservation

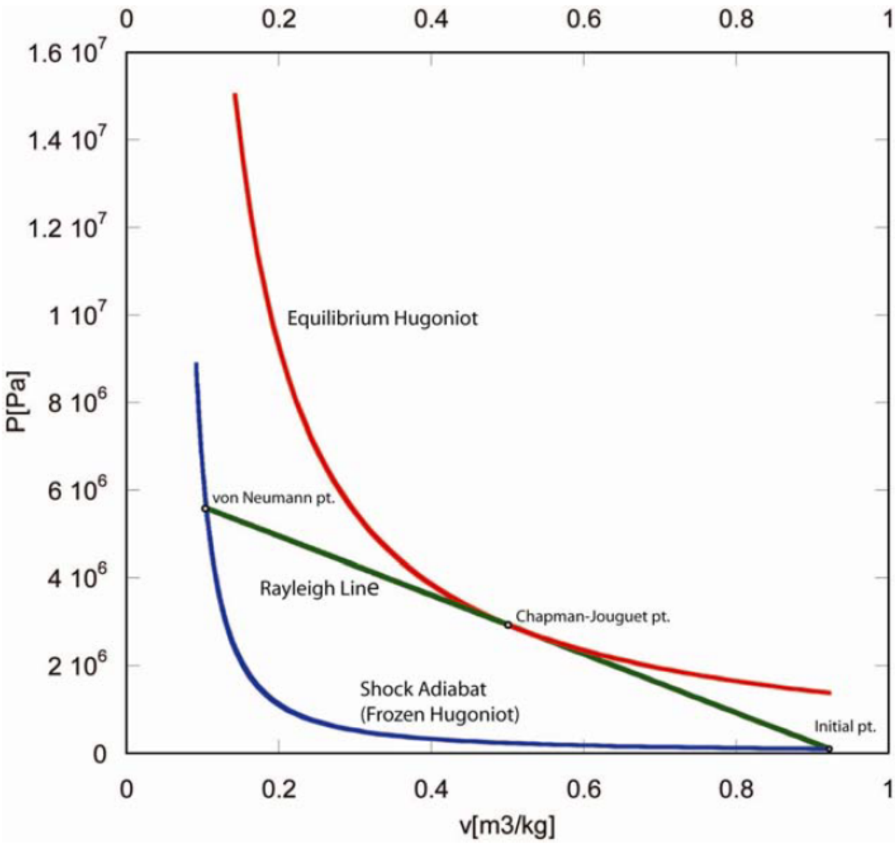

Figure 2: Rayleigh line and Hugoniot curves for Chapman-Jouguet methane/oxygen detonation

Equations used for calculations in SDToolbox:

$$p_2 = p_1 + \rho_1 u_1^2 (1 - \frac{\rho_1}{\rho_2}) \tag{1}$$

$$h_2 = h_1 + \frac{1}{2} u_1^2 (1 - \frac{\rho_1^2}{\rho_2^2}) \tag{2}$$

Equation which define Rayleight line:

$$p_2 = p_1 - \rho_1^2 u_1^2 (V_2 - V_1) \tag{3}$$

Equation which define Hugoniot curve:

$$h_2 = h_1 + \frac{1}{2}(p_2 - p_1)(V_2 + V_1) \tag{4}$$

0.3 Mathematical calculations of equivalence ratio

Chemical stoichiometry needed to find the equivalence ratio:

$$C_3H_8 + 5O_2 = 3CO_2 + 4H_2O$$

$$(F/A)_{stoichiometric} = \frac{1}{5} = 0.2$$

$$\phi = \frac{F/A}{(F/A)_{stoichiometric}}$$

$$F/A = \phi * (F/A)_{stoichiometric}$$

$$A = \frac{F}{\phi * (F/A)_{stoichiometric}}$$

In the program I will assume constant number of propane moles, so only amount of oxygen moles will be changing according to the equation above.

0.4 Boundary parameters used in the project

$$T_{min} = 293K$$

$$T_{max} = 900K$$

$$P_{min} = 1atm$$

$$P_{max} = 4atm$$

$$\phi_{min} = 0.1$$

$$\phi_{max} = 2$$

0.5 Plots and conclusions.

Results for constant equivalence ratio and temperature: figures from 3 to 6.

Results for constant equivalence ratio and pressure: figures from 7 to 10.

Results for constant pressure and temperature: figures from 11 to 14.

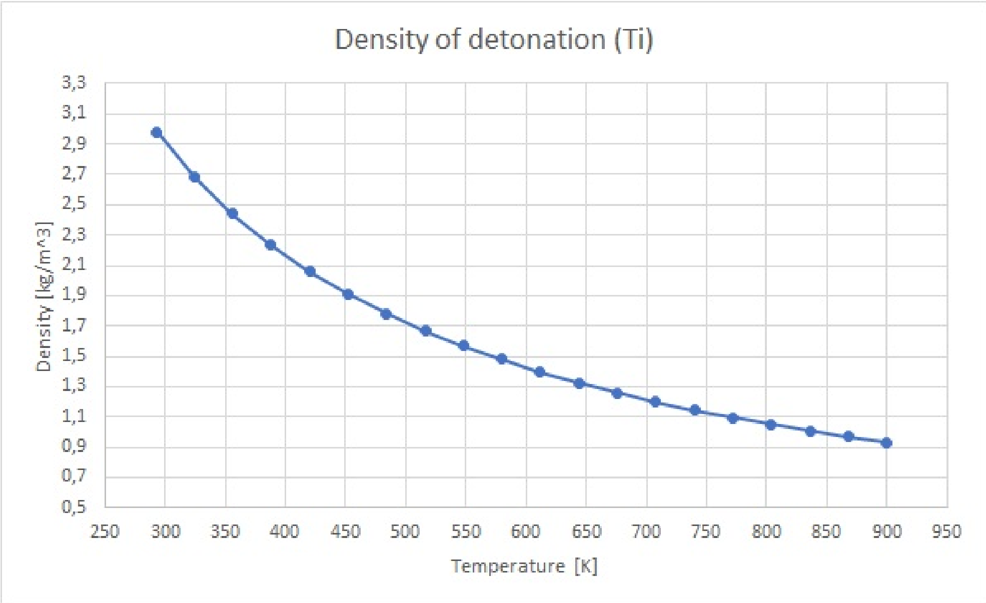

Figure 3: Detonation density in function of initial temperature.

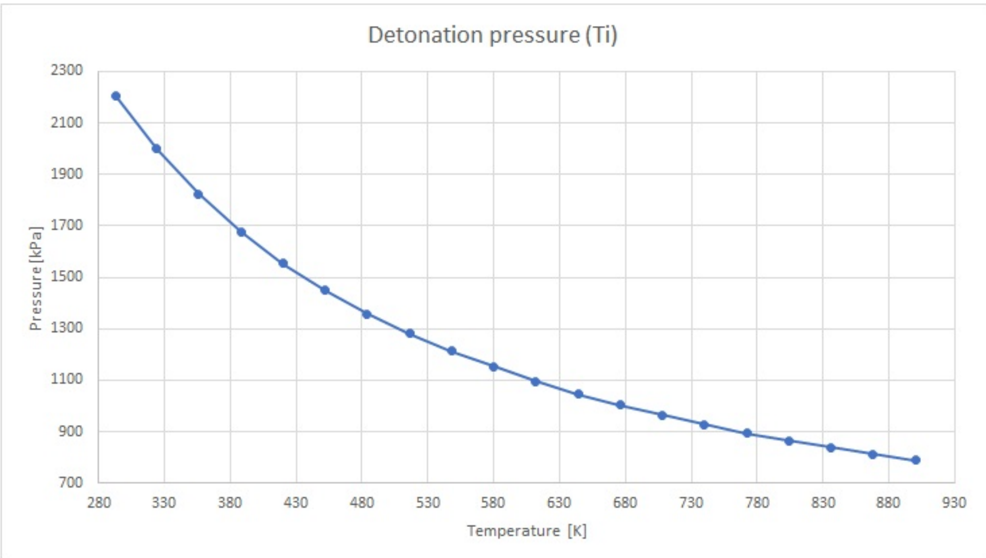

Figure 4: Detonation pressure in function of initial temperature.

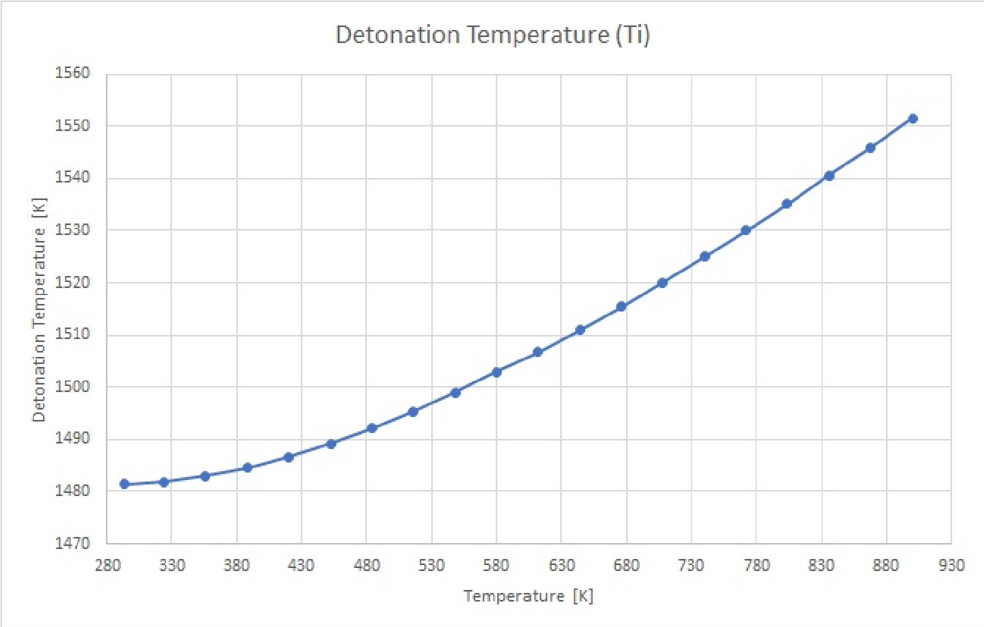

Figure 5: Detonation temperature in function of initial temperature.

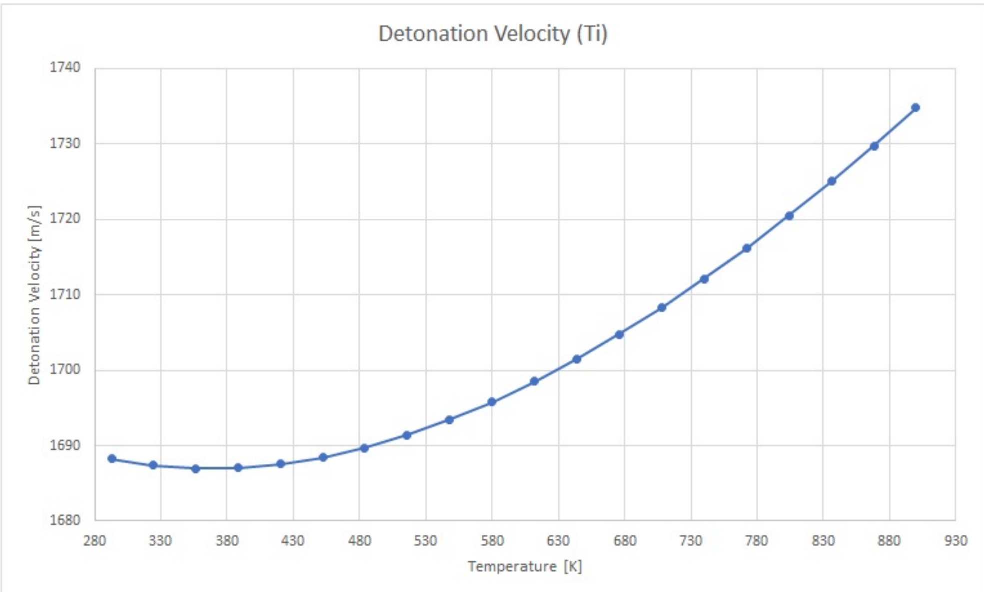

Figure 6: Detonation speed in function of initial temperature.

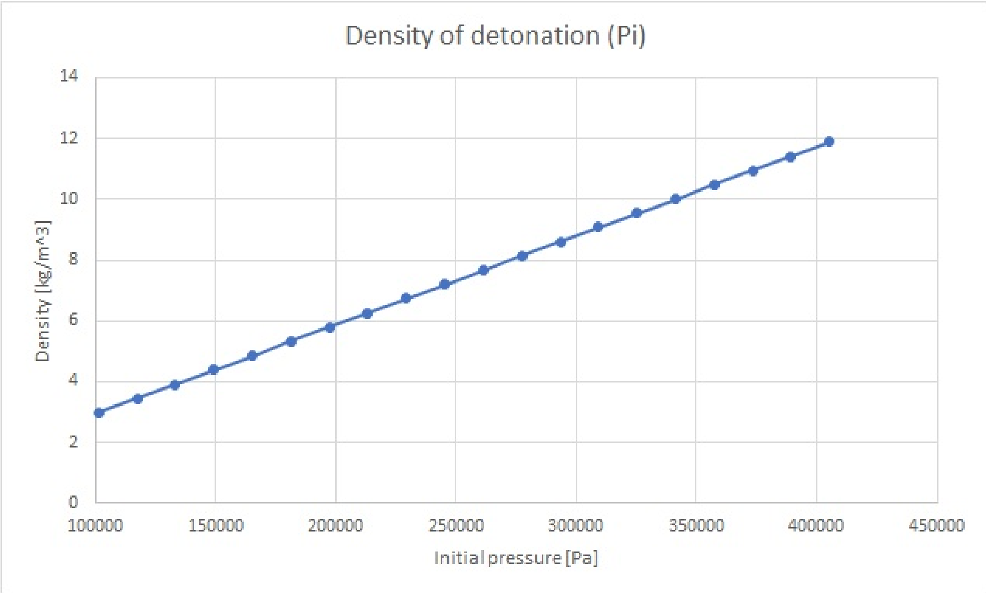

Figure 7: Detonation density in function of initial pressure.

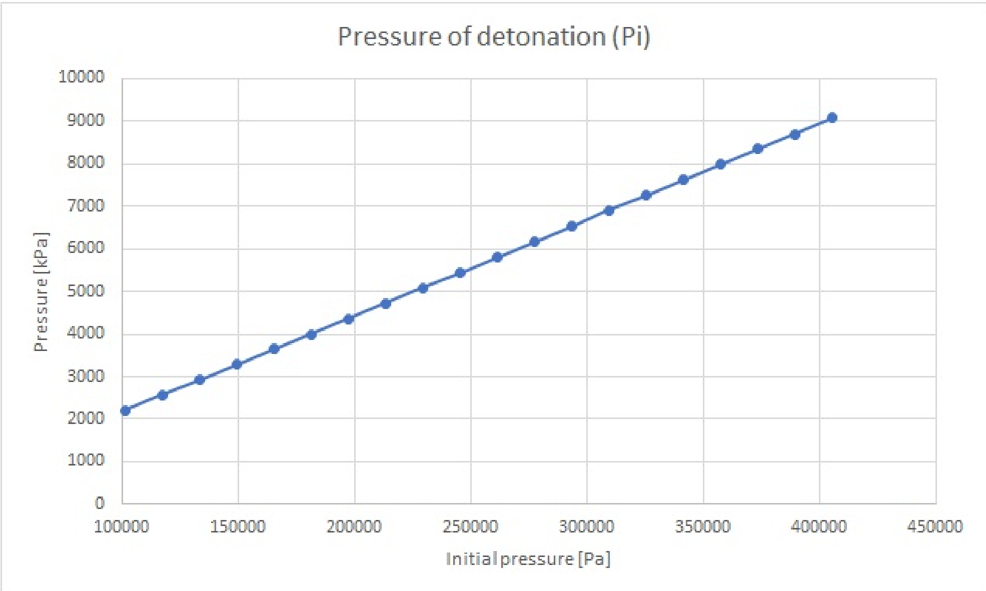

Figure 8: Detonation pressure in function of initial pressure.

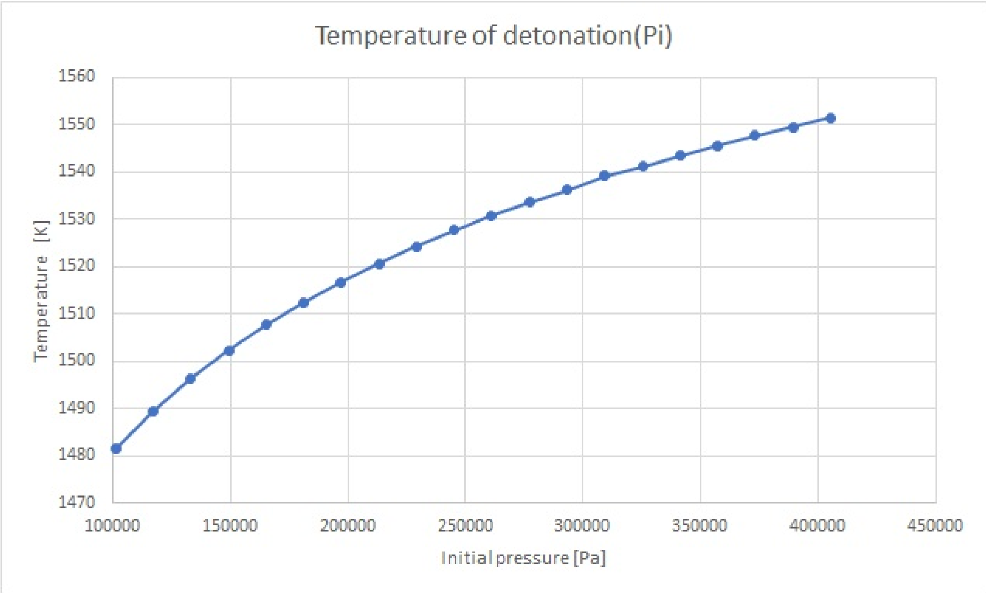

Figure 9: Detonation temperature in function of initial pressure.

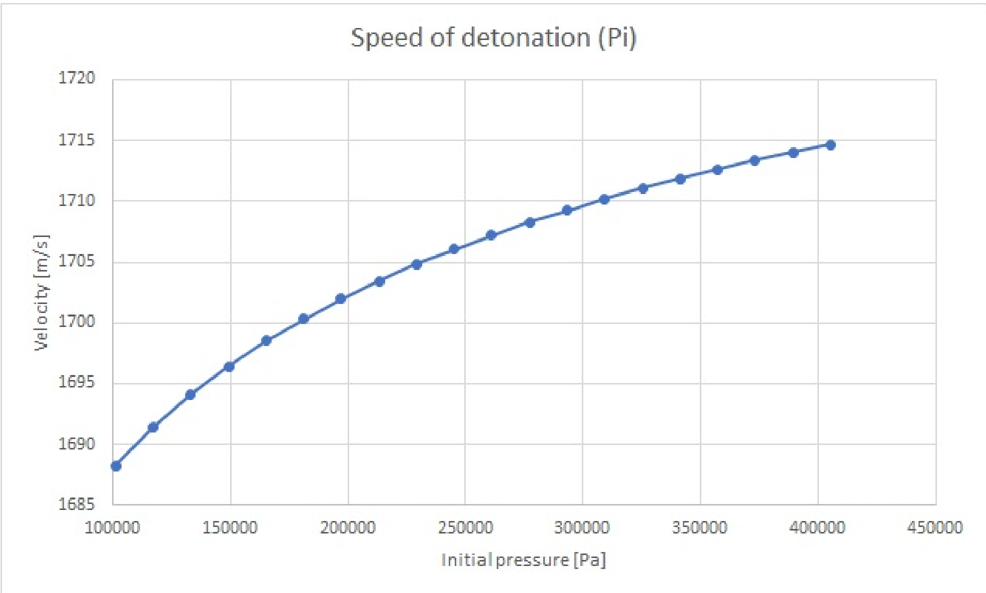

Figure 10: Detonation speed in function of initial pressure.

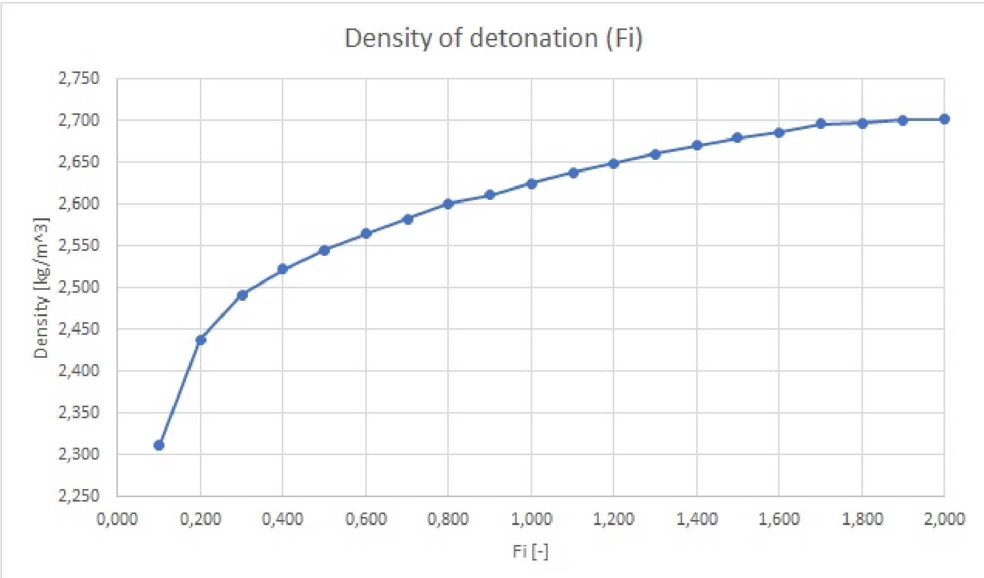

Figure 11: Detonation density in function of initial equivalence ratio.

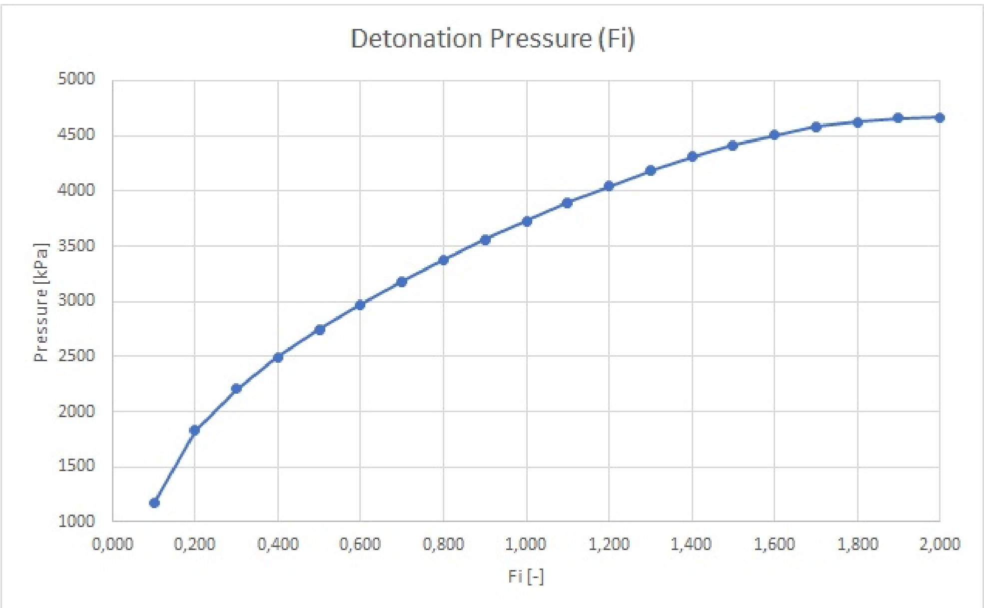

Figure 12: Detonation pressure in function of initial equivalence ratio.

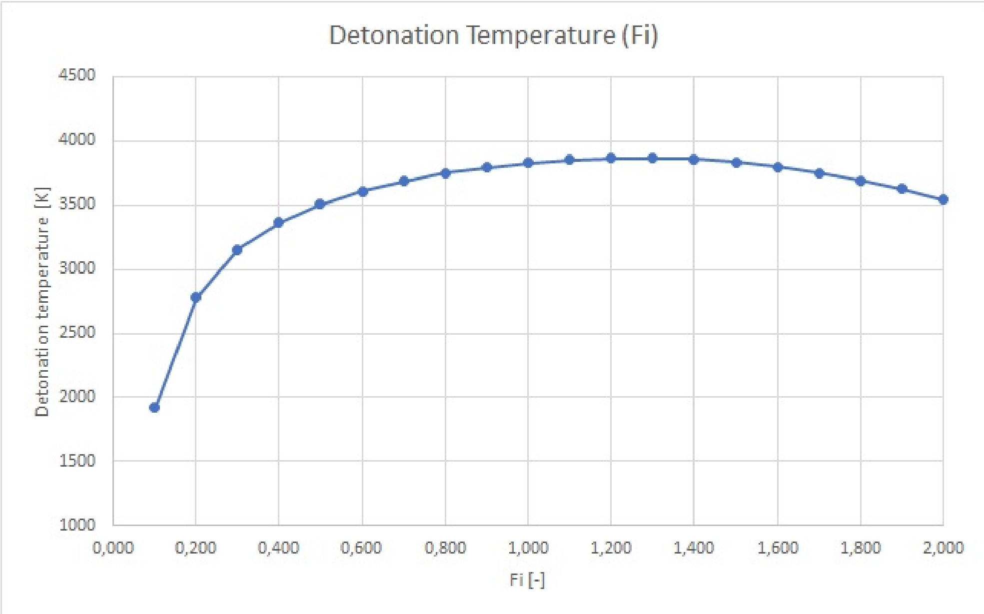

Figure 13: Detonation temperature in function of initial equivalence ratio.

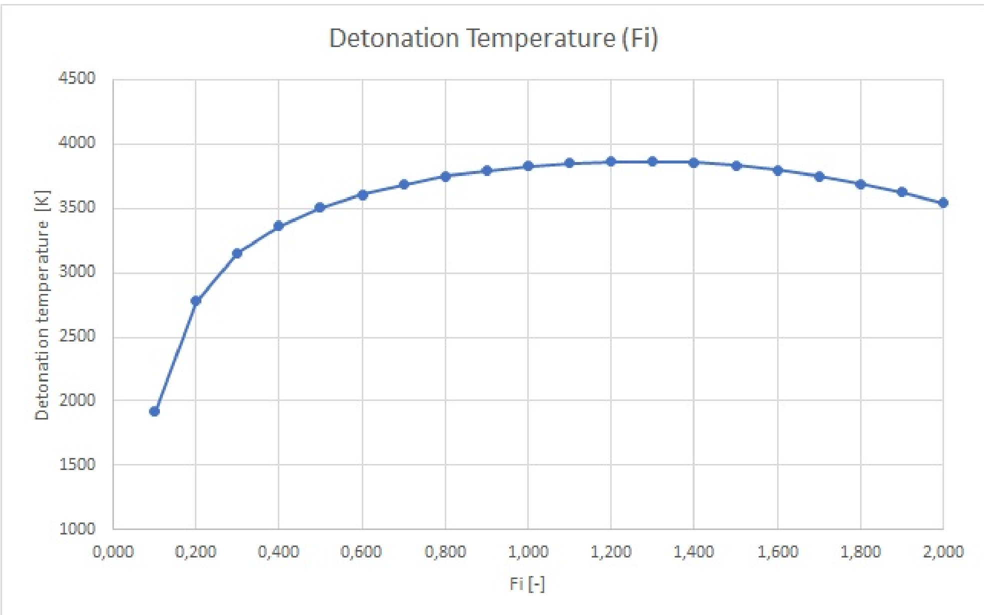

Figure 14: Detonation speed in function of initial equivalence ratio.

0.6 Charts descriptions

0.6.1 Detonation parameters in function of temperature.

Density is decreasing (from 2.98 kg/m^3 to 0.93 kg/m^3) and derivative is getting higher according to raising of the initial temperature.

Pressure, as it is in relation with density, is decreasing (from 2206 kPa to 790 kPa) and derivative is getting higher according to raising of the initial temperature.

Detonation temperature is increasing with growing initial parameter and its derivative is changing value at its beginning.

For detonation speed slight change is noticeable (from 1688 m/s^2 to 1735 m/s), where at the beginning its derivative is decreasing until initial temperature reach 388K.

0.6.2 Detonation parameters in function of pressure.

Density is increasing (from 2.98 kg/m^3 to 11.9 kg/m^3) and derivative is constant or almost constant according to raising of the initial pressure.

Detonation pressure, as it is in relation with density, is increasing (from 2206 kPa to 9074 kPa) and derivative is constant or almost constant according to raising of the initial temperature.

Detonation temperature is increasing with growing initial parameter and its derivative is getting smaller.

For detonation speed small change is noticeable (from 1688 m/s^2 to 1714 m/s), where at the beginning its derivative is decreasing.

0.6.3 Detonation parameters in function of equivalence ratio.

Density is increasing from 2.31 kg/m^3 to 2.7 kg/m^3) and derivative is getting smaller, close to value 0.

Pressure, as it is in relation with density, is increasing (from 1167 kPa to 4665 kPa) and derivatives is getting smaller, close to value 0.

Detonation temperature is increasing from fi=0.1 until fi=1.3 and after that point it is getting down.

The change of speed is way more noticeable than if was with other two initial parameters (from 1375 m/s^2 up to 2610 m/s), where derivative is decreasing until it almost reach the value of 0.

Bibliography

[1] Anne Felden *CANTERA Tutorials*

[2] Tetsu Nakamura *COMPUTATIONAL ANALYSIS OF ZEL'DOVICH-VON NEUMANN-DOERING (ZND) DETONATION*