The Faculty of Power and Aeronautical Engineering

Warsaw University of Technology

Computational Method in Combustion

Detonation velocity at various initial conditions for different mixtures

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Contents

1 Introduction

The goal of this project is to compare detonation velocity changes for the following three mixtures:

- Hydrogen (H_2)
- Methane (CH_4)
- Propane (C_3H_8)

at varying initial conditions. The tool that was used to perform calculations for this paper was SDToolbox under Cantera.

2 Theoretical model

The focal point of the project was to utilize Chapman-Jouguet (CJ) detonation. The CJ solution is used to approximate properties of an ideal steady detonation wave. Mass, momentum and energy preservation apply, as shown by the following equations:

- $\rho_1 h_1 = \rho_2 h_2$
- $P_1 + \rho_1 w_1^2 = P_2 + \rho_2 w_2^2$
- $h_1 + w_1^2/2 = h_2 + w_2^2/2$

The stoichiometric reactions of complete combustion of hydrogen, methane and propane in oxygen are as follows:

$$
\begin{gathered}
2\,\mathrm{H_2} + \mathrm{O_2} \longrightarrow 2\,\mathrm{H_2O} \\
\mathrm{CH_4} + 202 \longrightarrow 2\,\mathrm{H_2O} + \mathrm{CO_2} \\
\mathrm{C_3H_8} + 5\,\mathrm{O_2} \longrightarrow 3\,\mathrm{CO_2} + 4\,\mathrm{H_2O}
\end{gathered}
$$

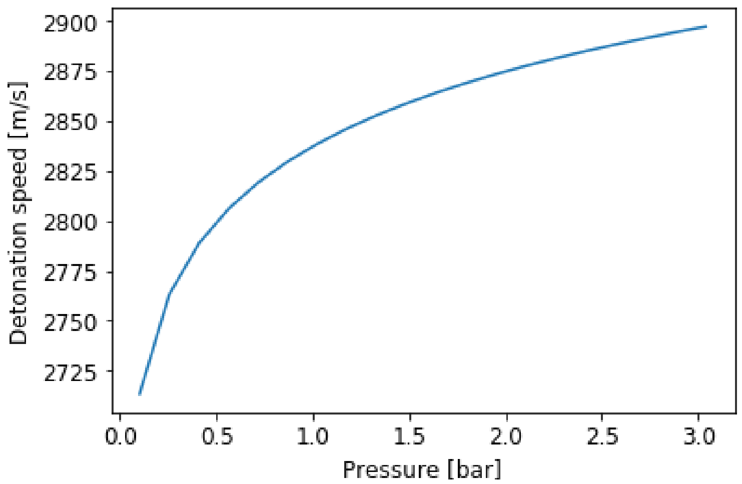
3 Code description

The project is based on calculations, using Python with the implementation of SDToolbox under Cantera.
Six different cases were considered for each mixture:

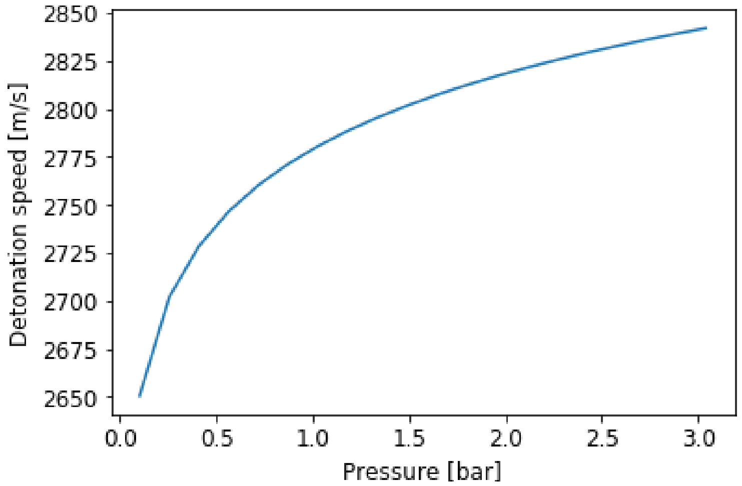
- I: v(p) at the initial temperature of 295 K,
- II: v(p) at the initial temperature of 500 K,
- III: v(p) at the initial temperature of 1000 K,
- IV: v(T) at the initial pressure of 1atm,
- V: v(T) at the initial pressure of 5atm,
- VI: v(T) at the initial pressure of 10atm,

4 Results

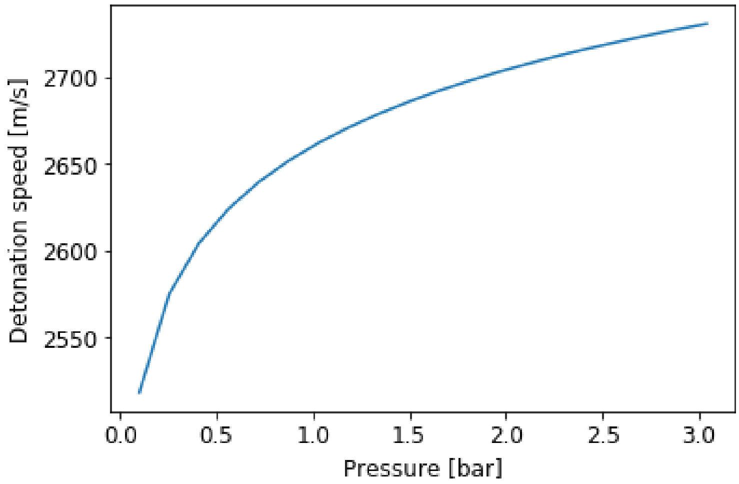
4.1 H_2, v(p)



Detonation velocity of hydrogen in relation to pressure, initial T=295K

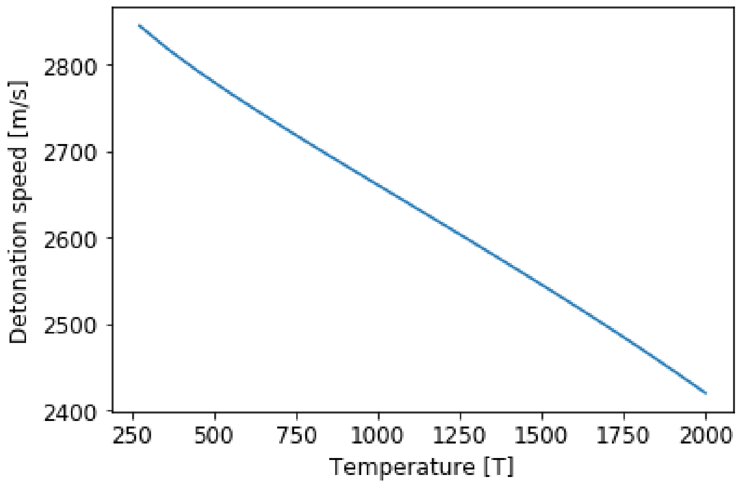


Detonation velocity of hydrogen in relation to pressure, initial T=500K

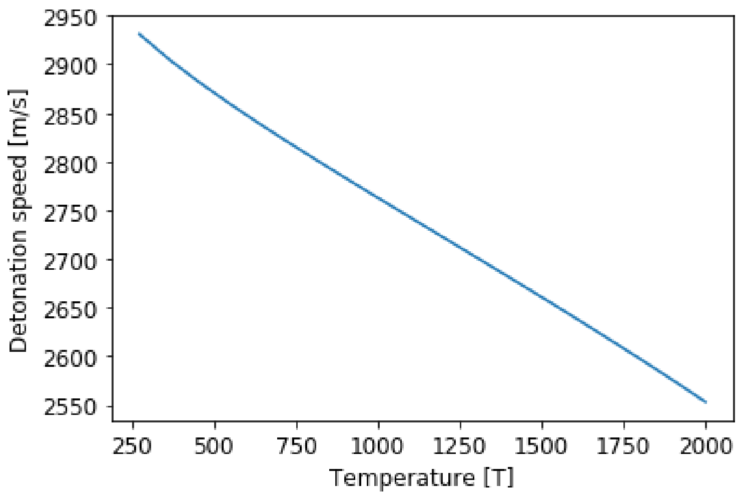


Detonation velocity of hydrogen in relation to pressure, initial T=1000K

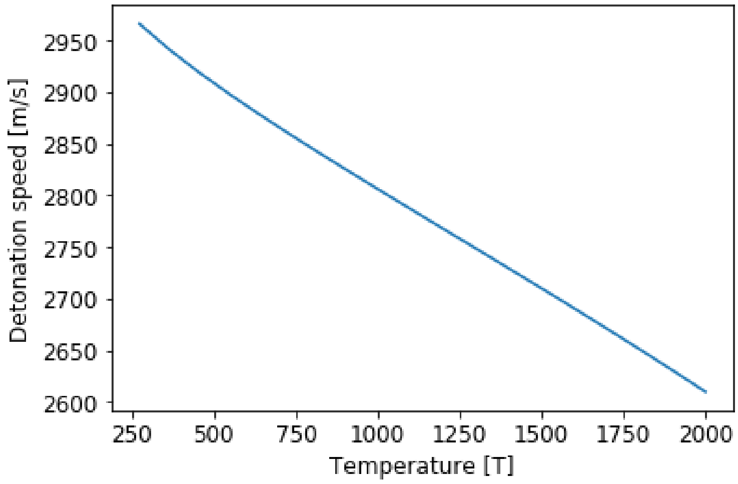
4.2 H_2, v(T)



Detonation velocity of hydrogen in relation to temperature, initial p=1atm

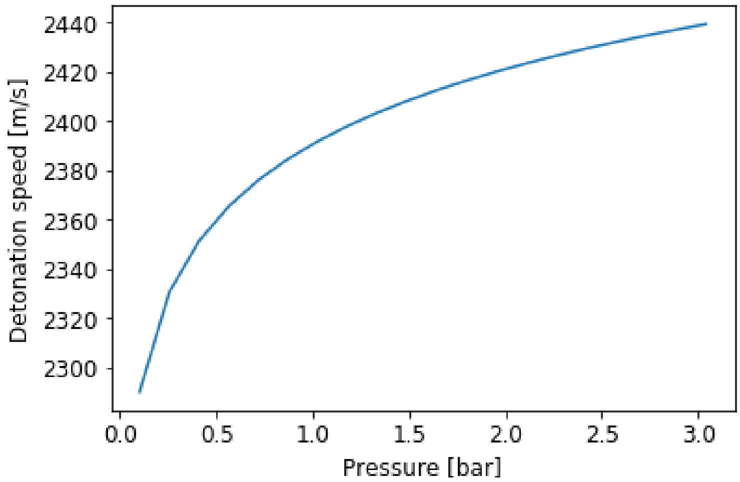


Detonation velocity of hydrogen in relation to temperature, initial p=5atm

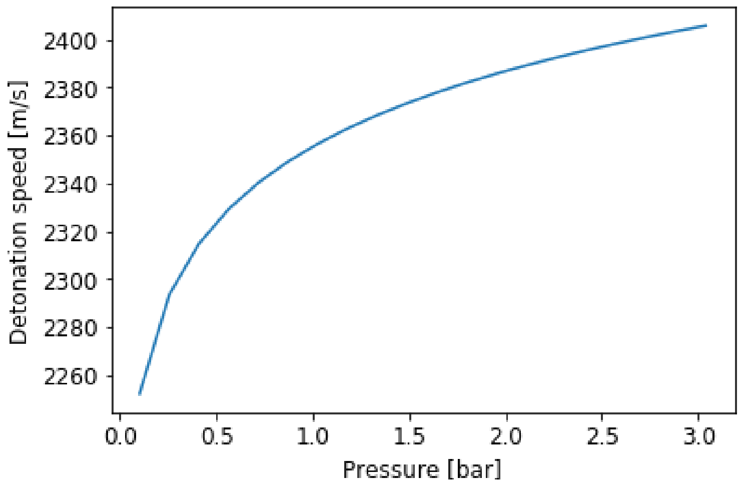


Detonation velocity of hydrogen in relation to temperature, initial p=10atm

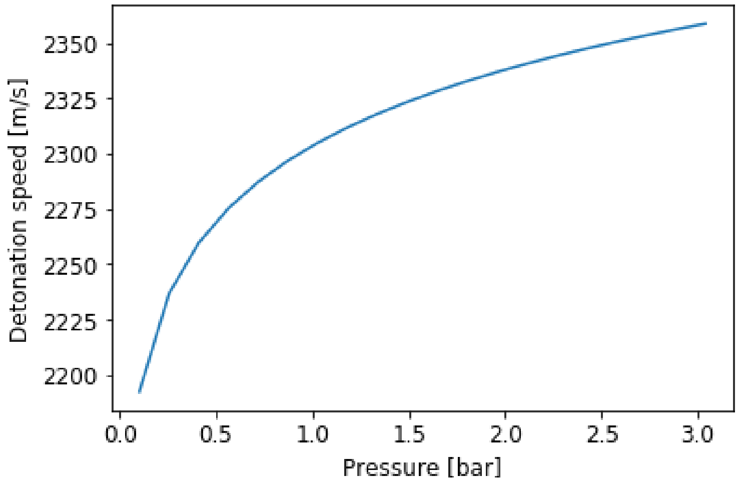
4.3 CH_4, v(p)



Detonation velocity of methane in relation to pressure, initial T=295K

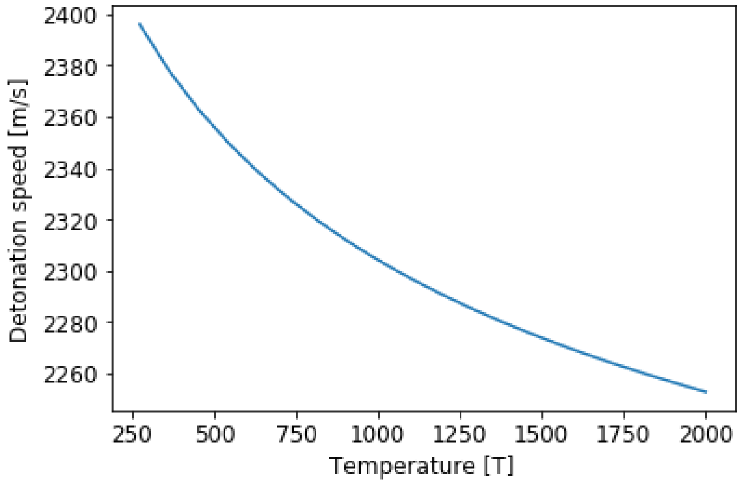


Detonation velocity of methane in relation to pressure, initial T=500K

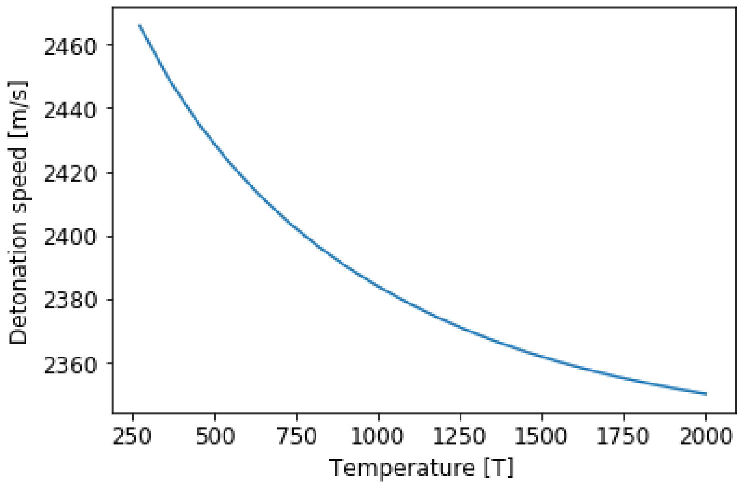


Detonation velocity of methane in relation to pressure, initial T=1000K

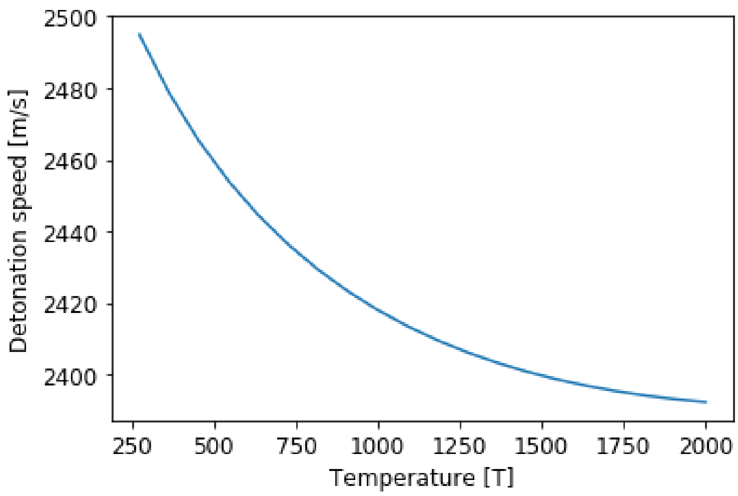
4.4 CH_4, v(T)



Detonation velocity of methane in relation to temperature, initial p=1atm

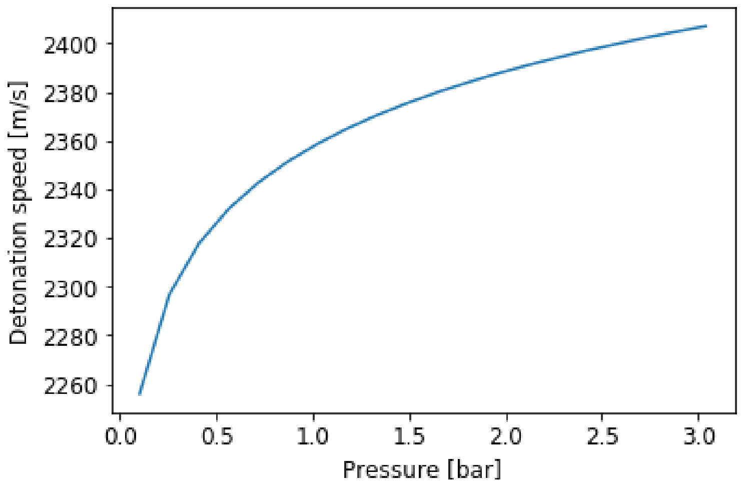


Detonation velocity of methane in relation to temperature, initial p=5atm

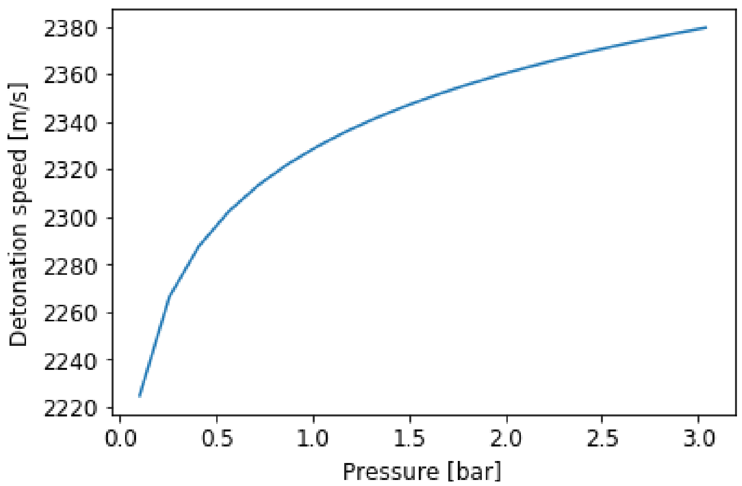


Detonation velocity of methane in relation to temperature, initial p=10atm

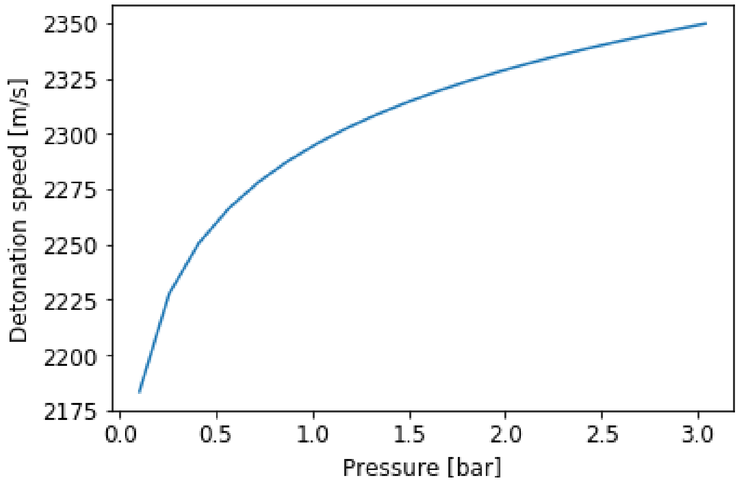
4.5 C_3H_8, v(p)



Detonation velocity of propane in relation to pressure, initial T=295K

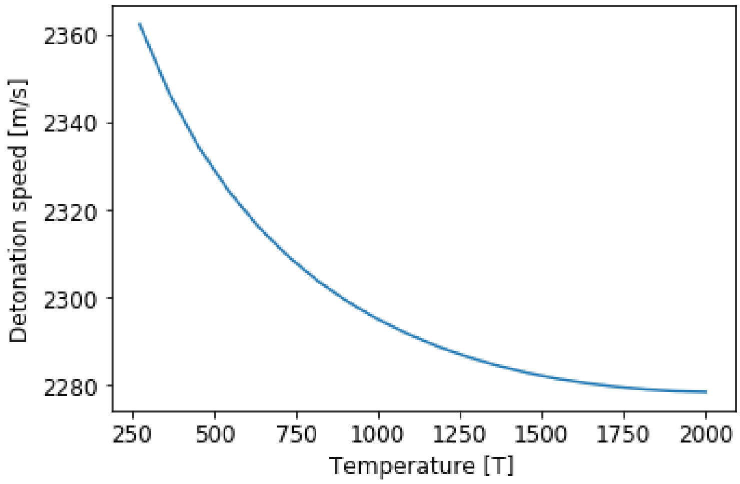


Detonation velocity of propane in relation to pressure, initial T=500K

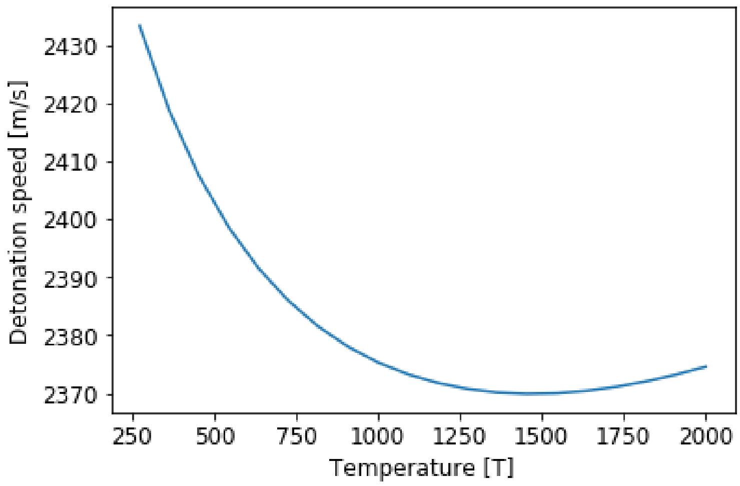


Detonation velocity of propane in relation to pressure, initial T=1000K

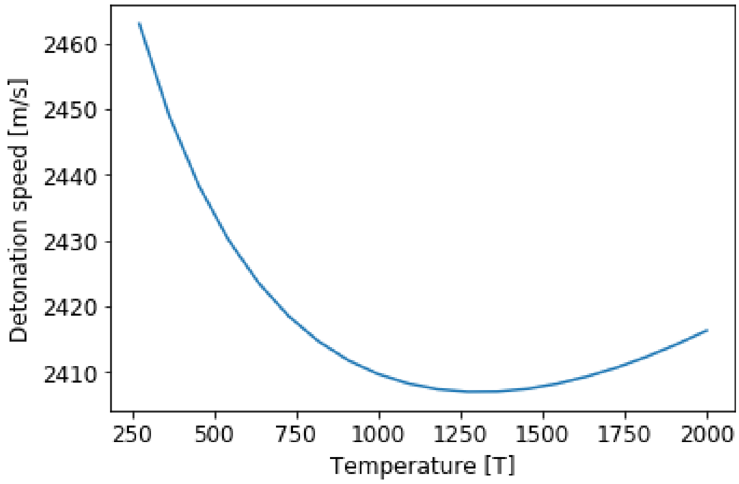
4.6 C_3H_8, v(T)



Detonation velocity of propane in relation to temperature, initial p=1atm



Detonation velocity of methane in relation to temperature, initial p=5atm



Detonation velocity of methane in relation to temperature, initial p=10atm

5 Summary

Analysis of the results is leading to following conclusions:

- The mixture of hydrogen and oxygen has the highest value of CJ speed and is the only one with a close-to-linear, decreasing tendency of detonation speed in relation to temperature.
- The detonation velocity for all mixtures considered is increasing with the rising pressure (logarithmic-esque curve).
- Initial conditions have an influence on detonation velocity.
- The higher the initial temperature, the lower the detonation speed for all mixtures considered.
- The higher the initial pressure, the higher the detonation speed for all mixtures considered

6 References

[1] http://shepherd.caltech.edu/EDL/publicresources.html
[2] https://github.com/BartoszBaszniak/MKWS/blob/master/MKWS
[3] https://cantera.org/examples/python/reactors/combustor.py.html
[4] http://combustion.berkeley.edu/gri-mech/version30/text30.html
[5] https://github.com/Bazyl29/MKWS/blob/master/Detonation