The Faculty of Power and Aeronautical Engineering

Warsaw University of Technology

Computational Methods in Combustion

Detonation velocity at various initial conditions for different mixtures

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1 Introduction

This project aims to compare detonation velocity changes for the following substances:

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

at various initial conditions. The calculations were performed with the use of SDToolbox.

2 Theoretical model

The project utilizes the Chapman-Jouguet (CJ) detonation model. The CJ model is used to approximate properties of an ideal steady detonation wave. Mass, momentum and energy preservation equations are:

$$\rho_1 h_1 = \rho_2 h_2$$

$$P_1 + \rho_1 \omega_1^2 = P_2 + \rho_2 \omega_2^2$$

$$h_1 + \omega_1^2/2 = h_2 + \omega_2^2/2$$

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

$$2H_2 + O_2 \rightarrow 2H_2O$$

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

$$C_3H_8 + 5O_2 \rightarrow 4H_2O + 3CO_2$$

3 Code description

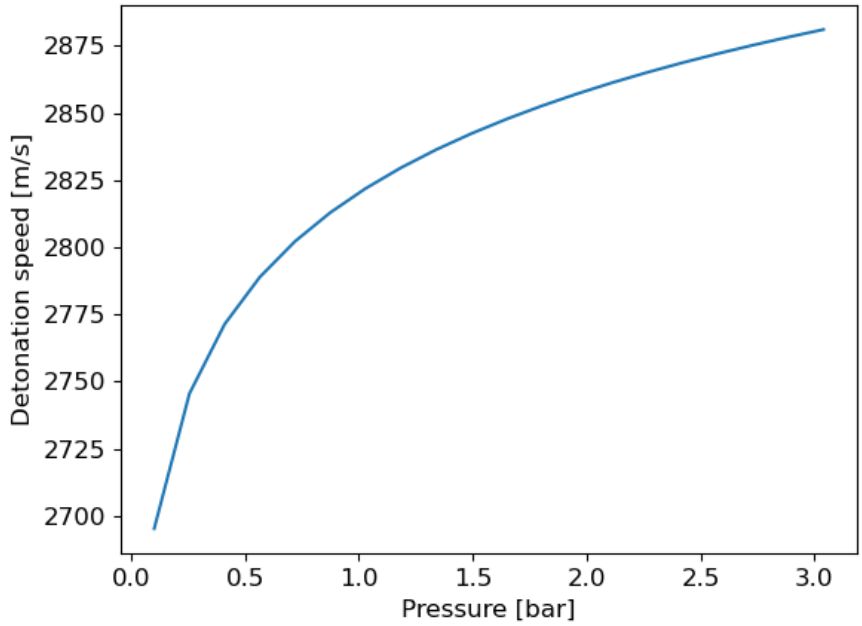
The project is based on calculations using Python with the implementation of SDToolbox. Calculations are preformed based on inserted initial conditions and substance. After the calculations are complete the results are plotted.

Six different cases were considered for each substance:

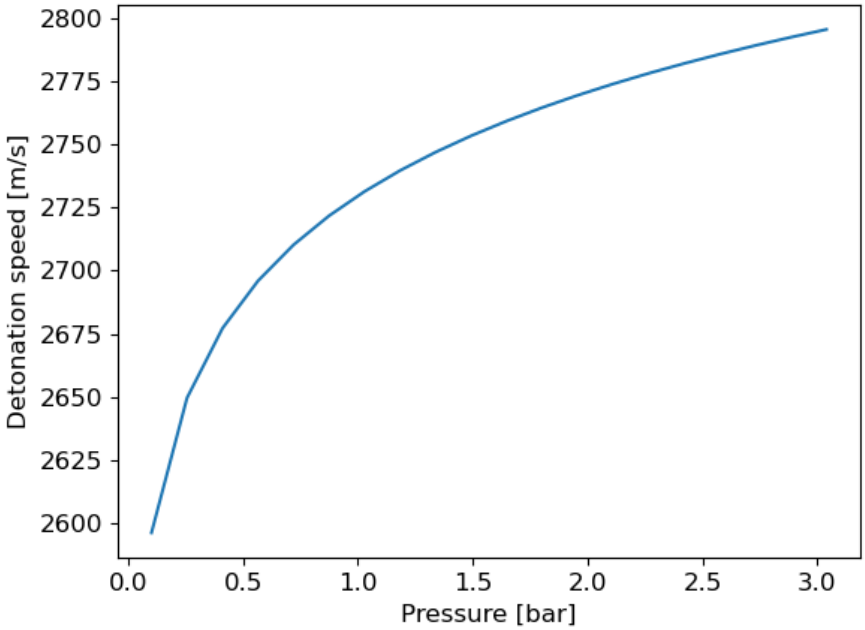
- I: v(p) at initial temperature of 350 K;
- II: v(p) at initial temperature of 700 K;
- III: v(p) at initial temperature of 1200 K;
- IV: v(T) at initial pressure of 2.5 atm;
- V: v(T) at initial pressure of 7.5 atm;
- VI: v(T) at initial pressure of 12.5 atm.

4 Results

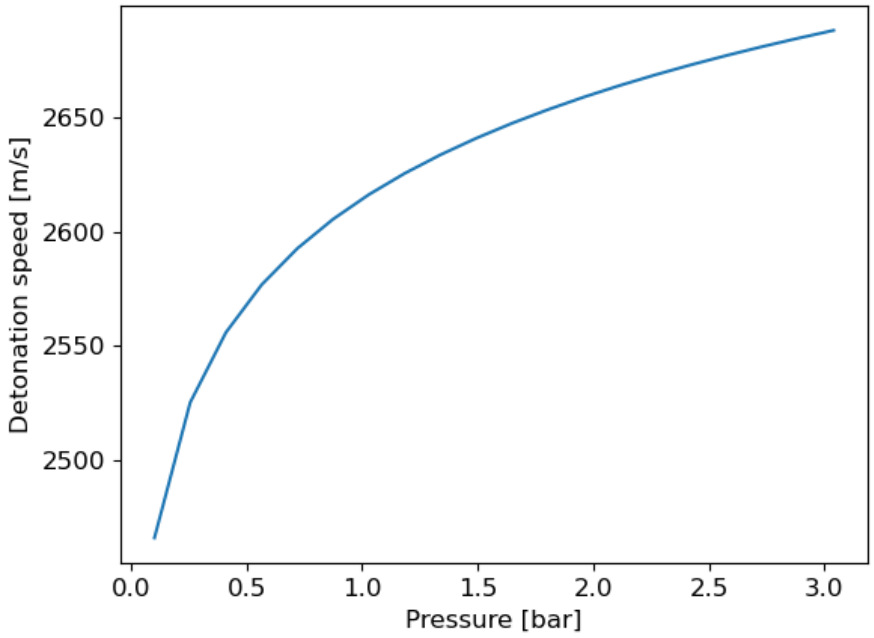
4.1 H_2, v(p)



Detonation velocity of hydrogen in relation to pressure, initial T = 350 K

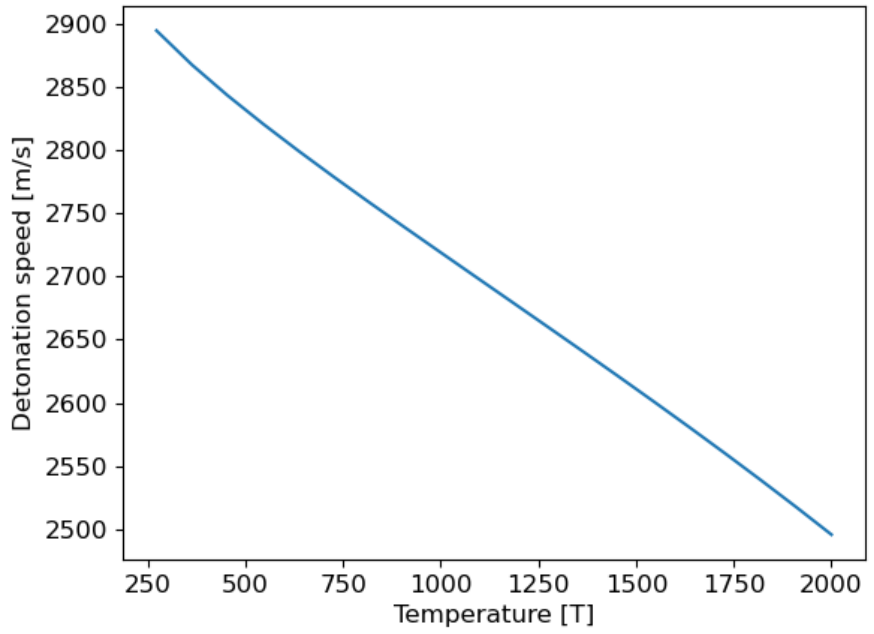


Detonation velocity of hydrogen in relation to pressure, initial T = 700 K

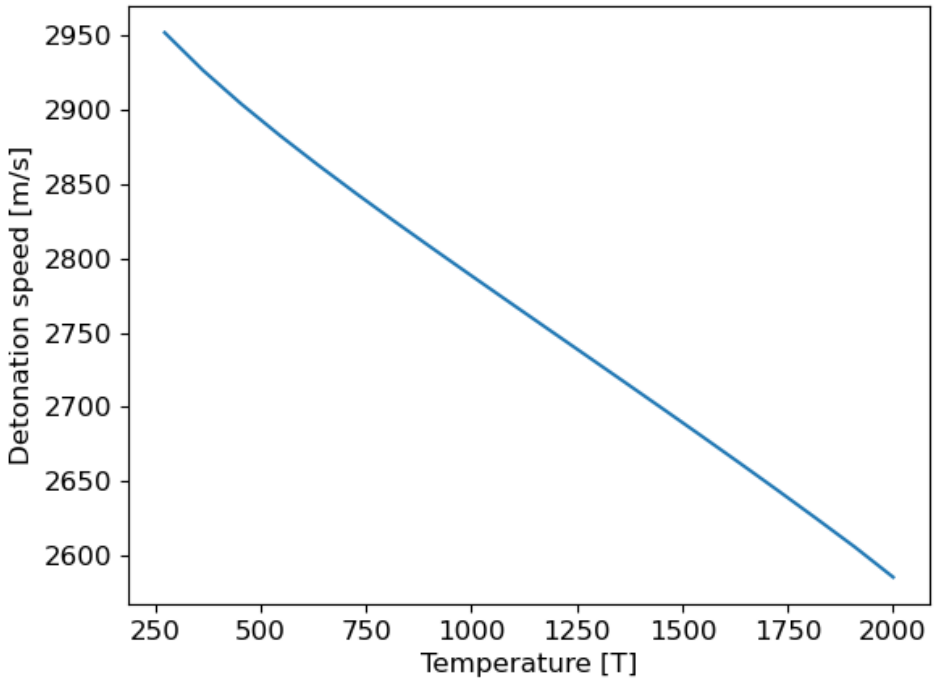


Detonation velocity of hydrogen in relation to pressure, initial T = 1200 K

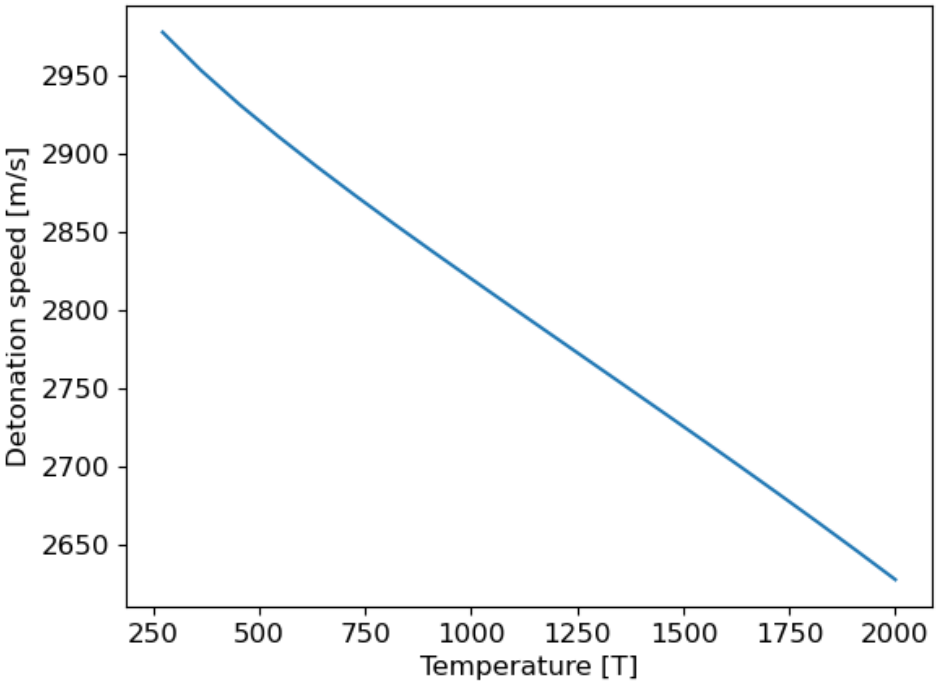
4.2 H_2, v(T)



Detonation velocity of hydrogen in relation to temperature, initial p = 2.5 atm

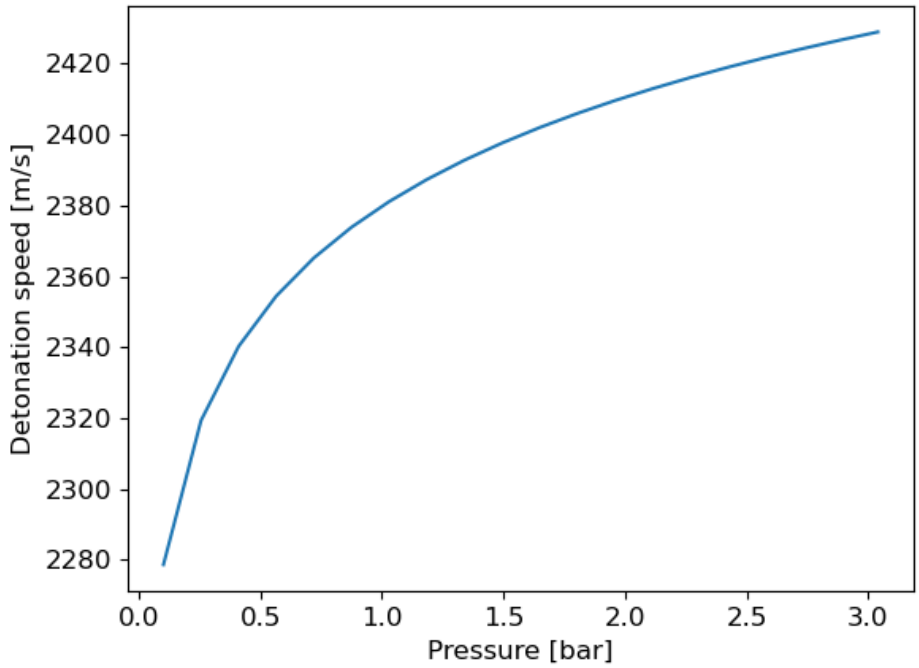


Detonation velocity of hydrogen in relation to temperature, initial p = 7.5 atm

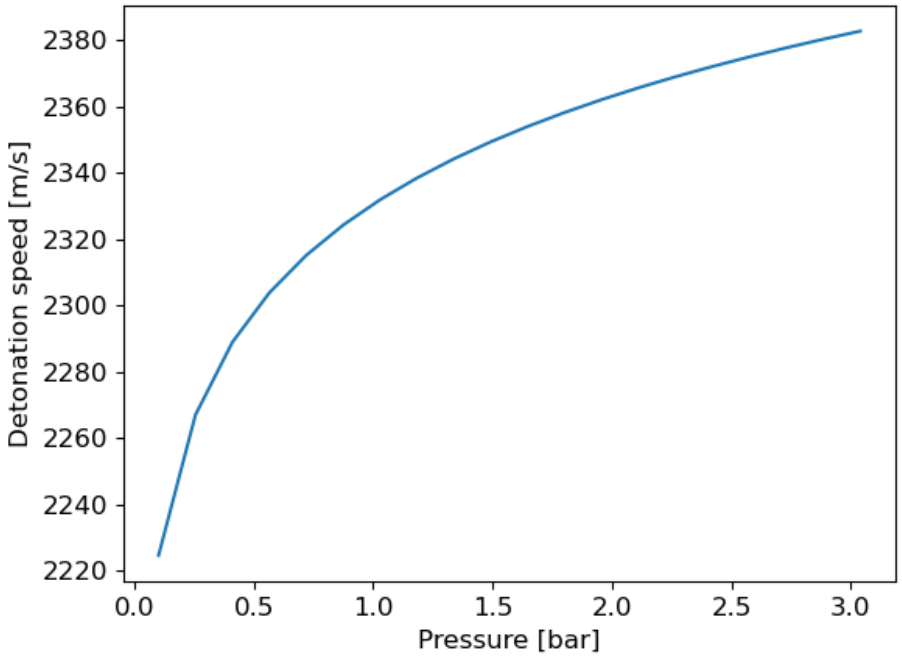


Detonation velocity of hydrogen in relation to temperature, initial p = 12.5 atm

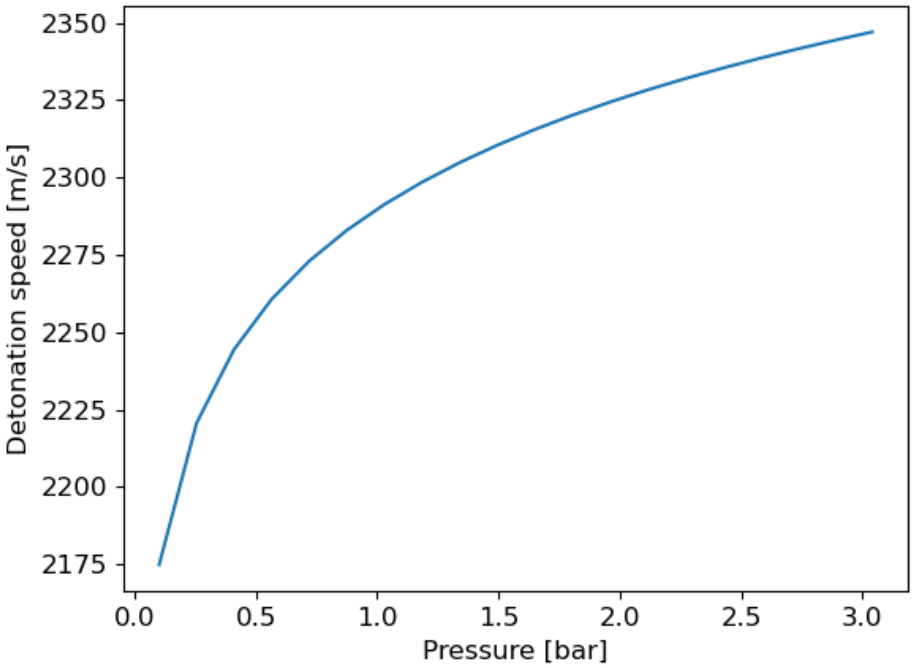
4.3 CH_4, v(p)



Detonation velocity of methane in relation to pressure, initial T = 350 K

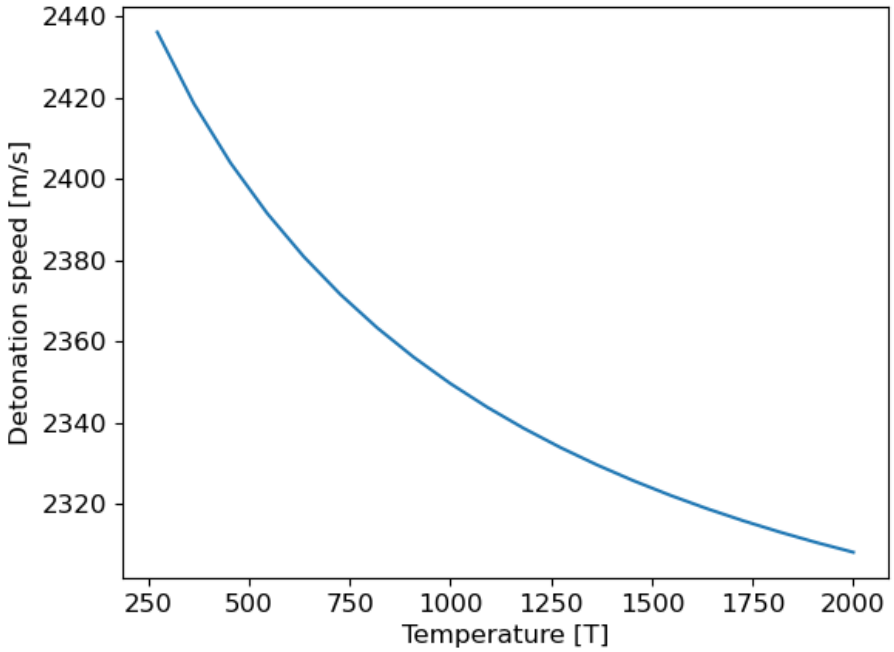


Detonation velocity of methane in relation to pressure, initial T = 700 K

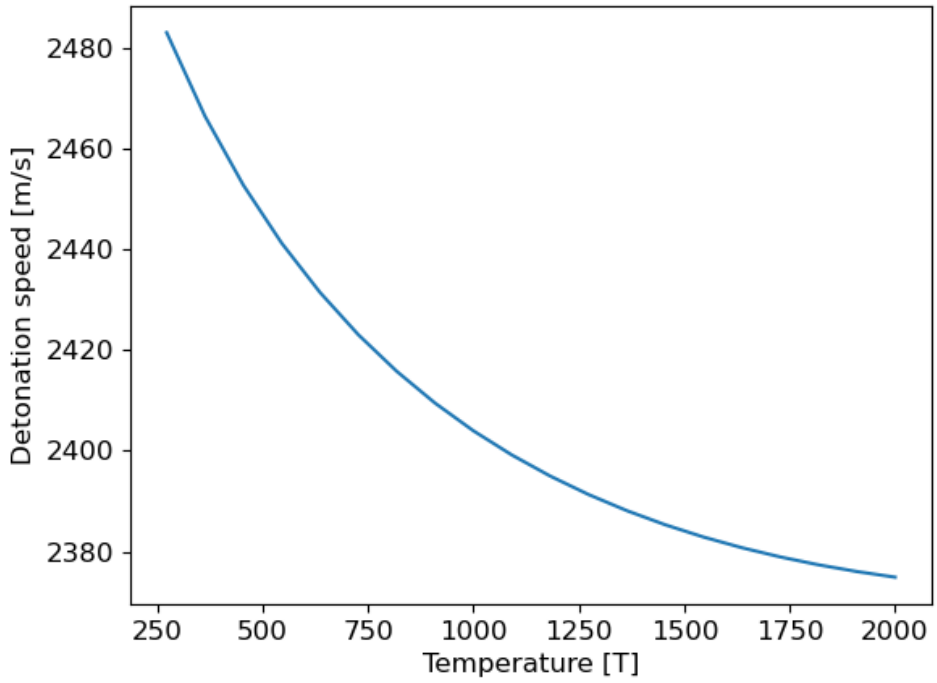


Detonation velocity of methane in relation to pressure, initial T = 1200 K

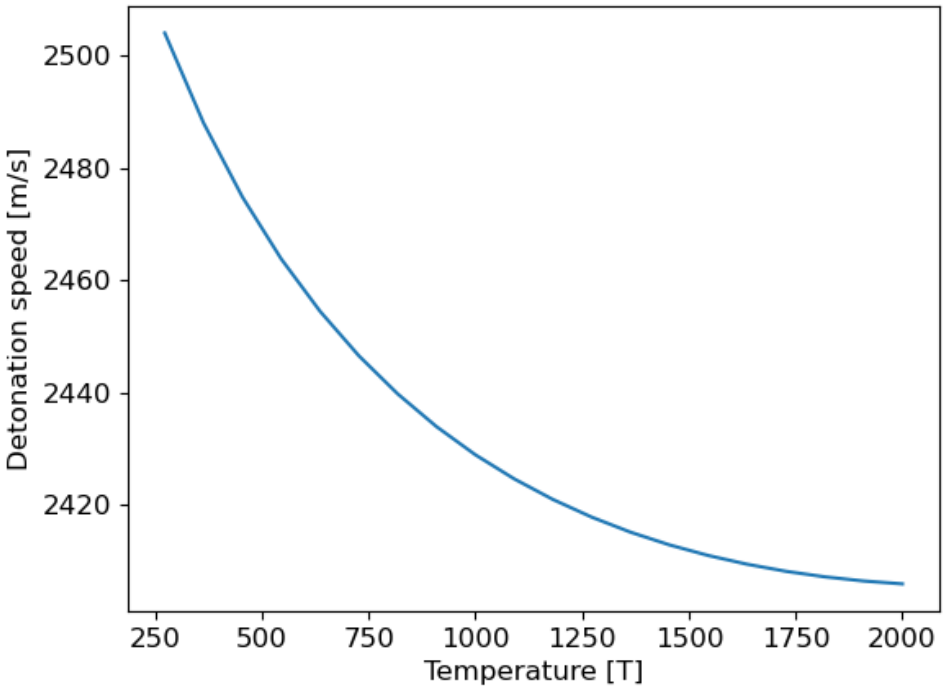
4.4 CH_4, v(T)



Detonation velocity of methane in relation to temperature, initial p = 2.5 atm

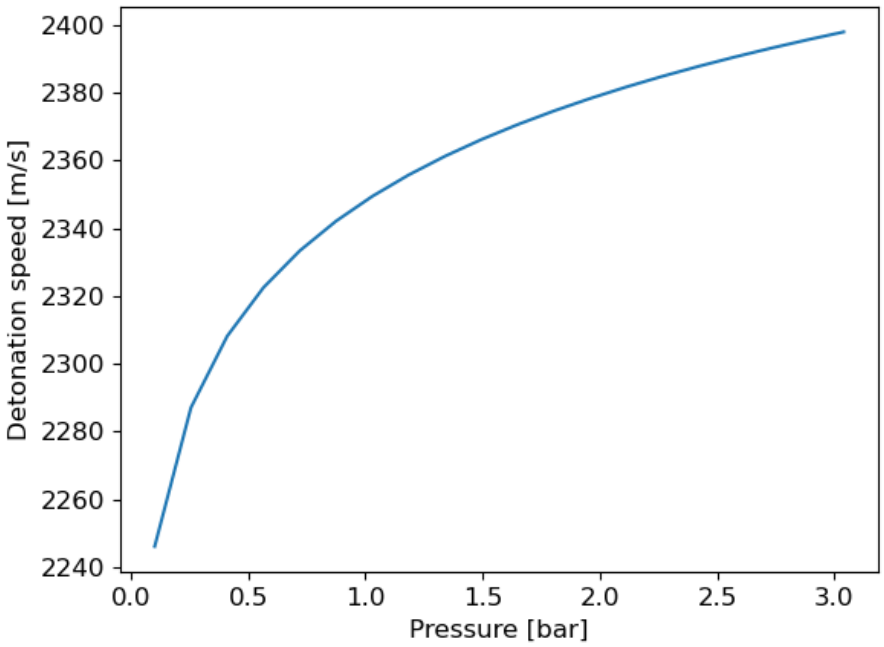


Detonation velocity of methane in relation to temperature, initial p = 7.5 atm

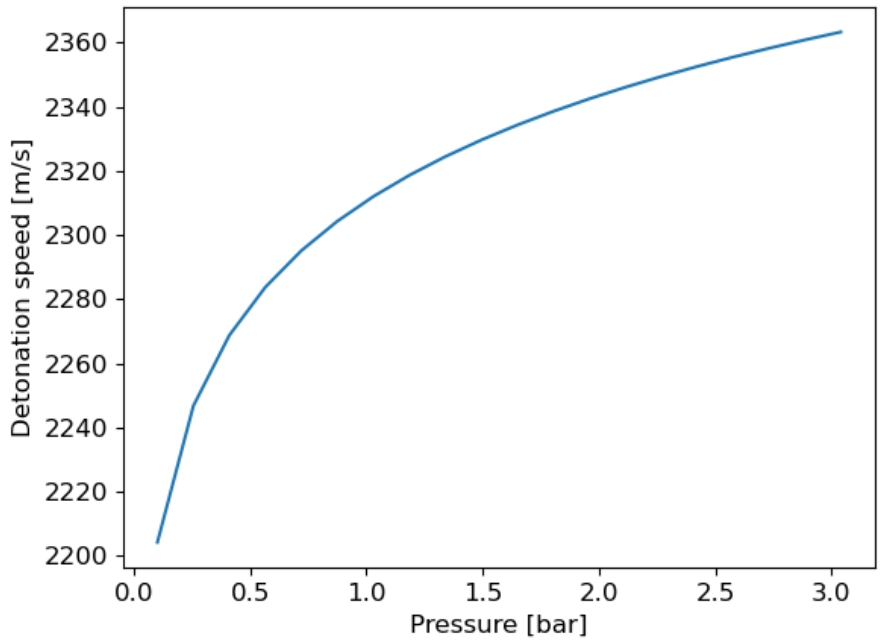


Detonation velocity of methane in relation to temperature, initial p = 12.5 atm

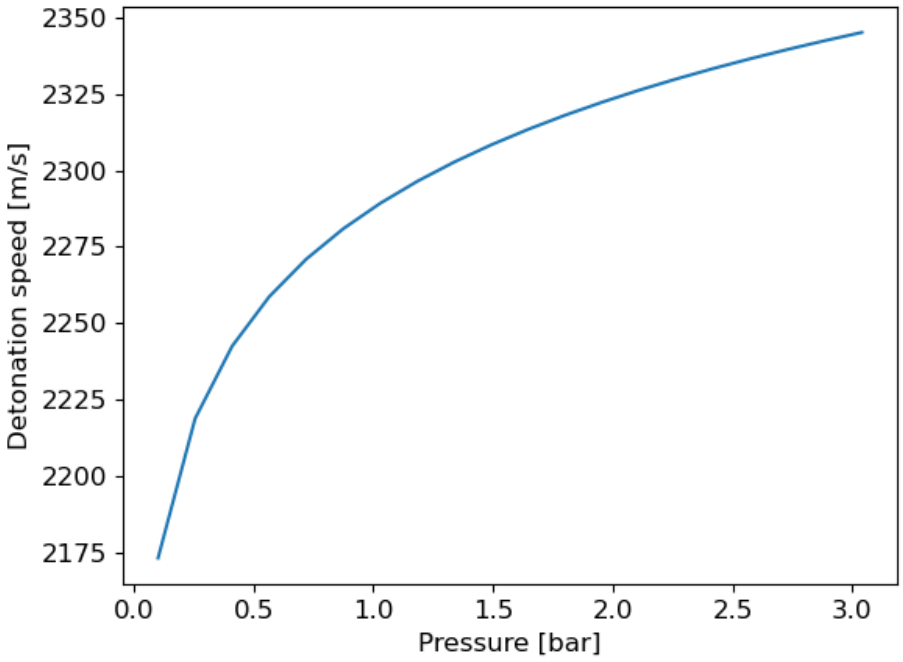
4.5 C_3H_8, v(p)



Detonation velocity of propane in relation to pressure, initial T = 350 K

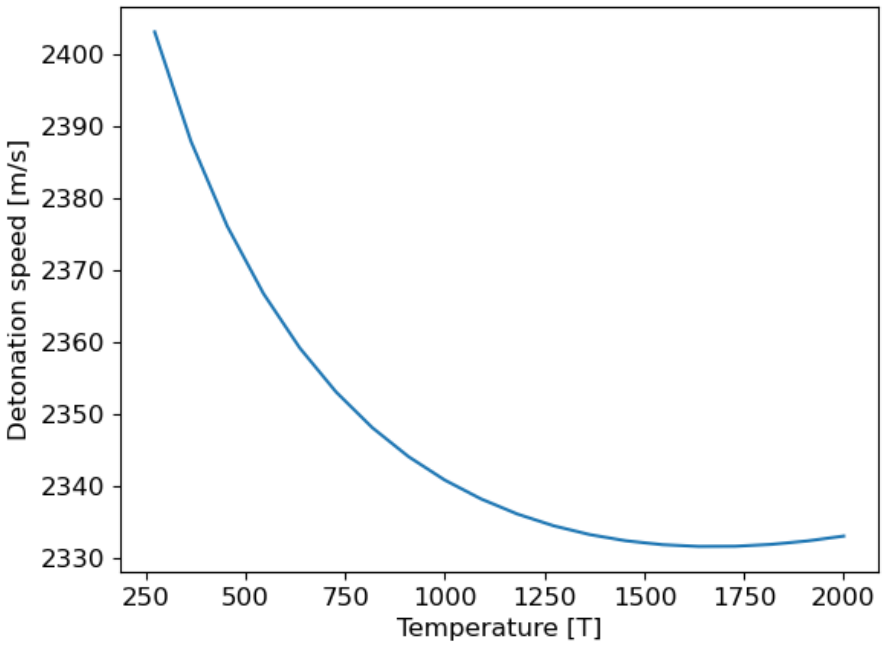


Detonation velocity of propane in relation to pressure, initial T = 700 K

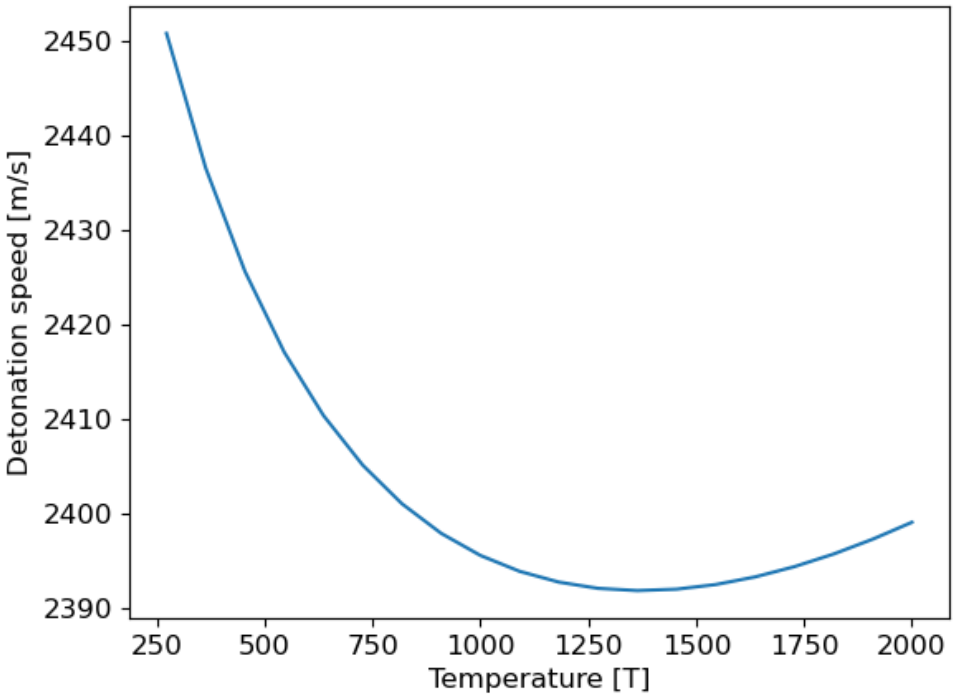


Detonation velocity of propane in relation to pressure, initial T = 1200 K

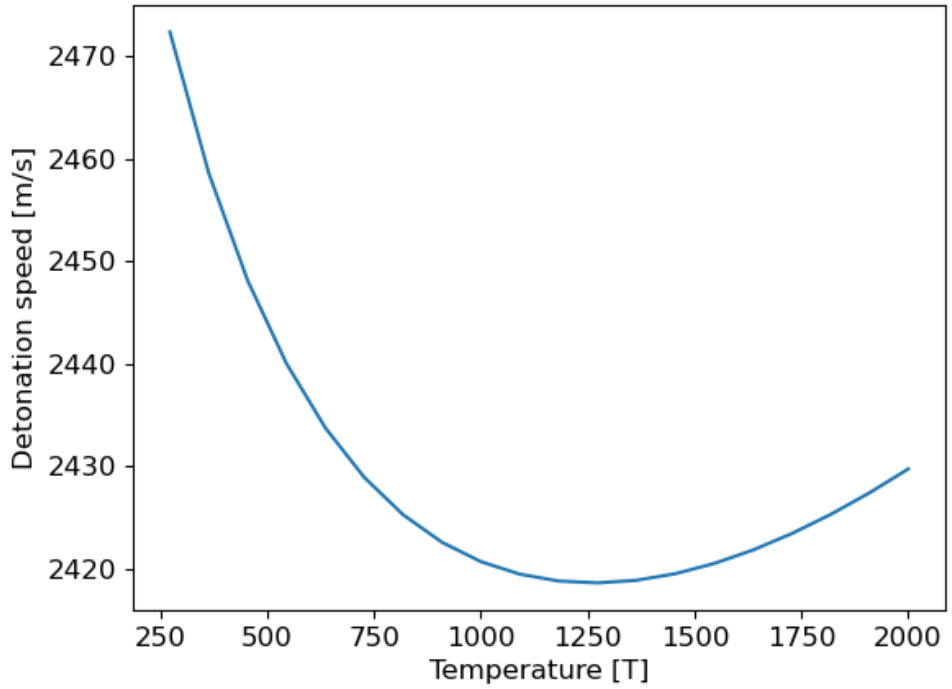
4.6 C_3H_8, v(T)



Detonation velocity of propane in relation to temperature, initial p = 2.5 atm



Detonation velocity of propane in relation to temperature, initial p = 7.5 atm



Detonation velocity of propane in relation to temperature, initial p = 12.5 atm

5 Summary

- The higher the initial pressure the higher the detonation speed for all substances considered;
- The higher the initial temperature the lower the detonation speed for all substances considered;
- The mixture of hydrogen and oxygen has the highest 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 substances considered is increasing in a logarithmic-like manner.

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