Warsaw University of Technology
Faculty of Power and Aeronautical Engineering

Computer Methods in Combustion

Calculation of the detonation velocity of the hydrogen-air mixture in a constant volume for variable initial parameters

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1 Introduction

Detonation is a compression wave propagating supersonically, which can be produced by driving a piston at an appropriate speed into the mixture. It compresses the burned gas, slowing it down. The downstream flow is:

- sonic ($M_2 = 1$) for Chapman-Jouguet detonation
- supersonic ($M_2 > 1$) for weak detonations
- subsonic ($M_2 < 1$) for strong detonations

Weak detonations can propagate only at one speed.

2 Theoretical background

2.1 Rankine-Hugoniot equations

Consider a mixture of combustible gases in a straight pipe of constant cross section in which we have a plane combustion wave propagating along the pipe axes. The wave is described in coordinate system stationary to the wave.

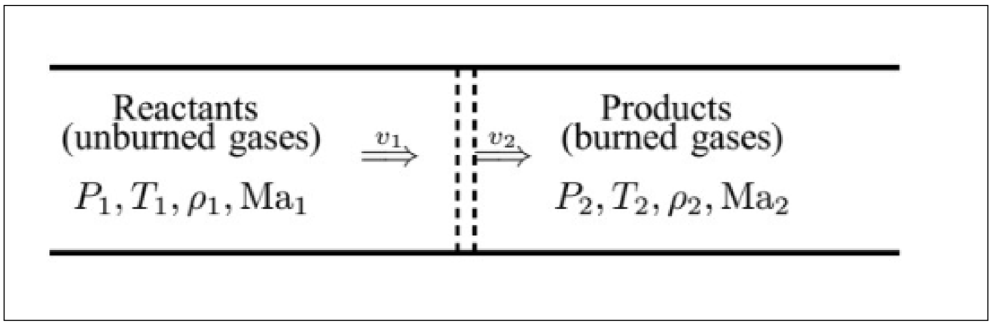

Figure 1: Detonation wave visualization

Than the mass, momentum and the energy preservation equations are:

$$\rho_1 v_1 = \rho_2 v_2 = m \tag{1}$$

$$P_1 + \rho_1 v_1^2 = P_2 + \rho_2 v_2 \tag{2}$$

$$h_1 + \frac{v_1^2}{2} = h_2 + \frac{v_2^2}{2} \tag{3}$$

Where h - enthalpy equals to:

$$h(T) = \Sigma Y_i h_{fi}^o + \Sigma Y_i \int_{T_o}^{T} c_{pi} dT \tag{4}$$

Taking into consideration the fact that:

$$p = \rho R T \tag{5}$$

Assume $c_{p1} = c_{p2} = c_p$ and q - heat combustion per mass unit of combustible mixture

$$\rho_1 v_1 = \rho_2 v_2 \tag{6}$$

$$P_1 + \rho_1 v_1^2 = P_2 + \rho_2 v_2 \tag{7}$$

$$c_p T_1 + \frac{v_1^2}{2} = c_p T_2 + \frac{v_2^2}{2} - q \tag{8}$$

$$\frac{p_1}{\rho_1 T_1} = \frac{p_2}{\rho_2 T_2} = \frac{\kappa - 1}{\kappa} c_p \tag{9}$$

After some manipulations and use of the equation of state to eliminate T:

$$\frac{p_2 - p_1}{\frac{1}{\rho_2} - \frac{1}{\rho_1}} = -m^2 - \textit{Rayleigh Line} \tag{10}$$

$$\frac{\kappa}{\kappa - 1}\left(\frac{p_2}{\rho_2} - \frac{p_1}{\rho_1}\right) - 0.5\left(\frac{1}{\rho_2} + \frac{1}{\rho_1}\right)(p_2 - p_1) = q - \textit{Hugoniot curve} \tag{11}$$

By drawing the Rayleigh Line and the Hugoniot curve on the same plot allows to visualize solutions of above equations:

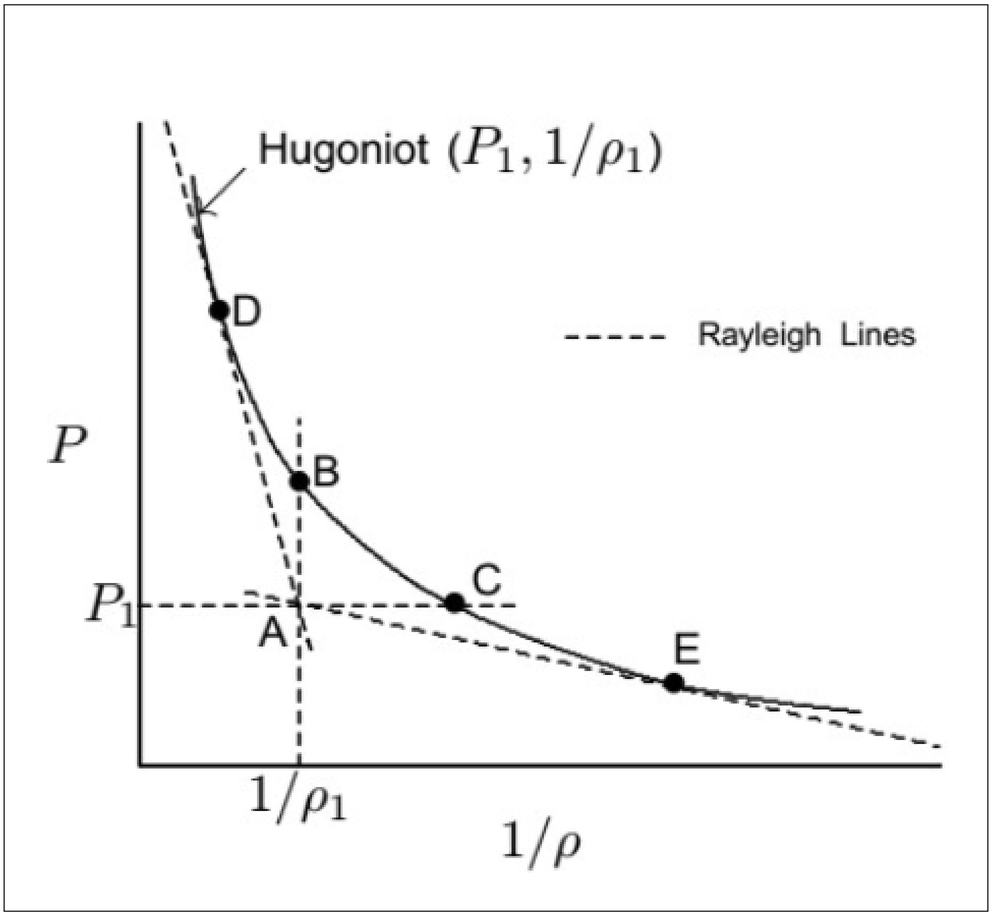

Figure 2: Rankine-Hugoniot curve

As we can see, four Rayleigh Lines divide a Hugoniot curve into five regions:

- above point D - strong detonation
- B-D - weak detonation
- C-E - weak deflagration
- below point E - strong deflagration

2.2 Chapman-Jouguet detonation

The Chapman-Jouguet (C-J) detonation is a detonation, where the outlet gas velocity is sonic. Assuming constant heat capacities of the reactants and transforming mass, momentum and energy conservation equations the detonation velocity may be calculated as:

$$v_{C-J} = \sqrt{2(\kappa_2^2 - 1)(q + c_{p1}T_1)} \tag{12}$$

In the Figure 2 Chapman - Jouguet detonation is represented by the point D.

2.3 ZND detonation model

ZND detonation model is a developed C-J model that takes into consideration the finite time of the reaction. Due to that theory the structure of the detonation looks as below:

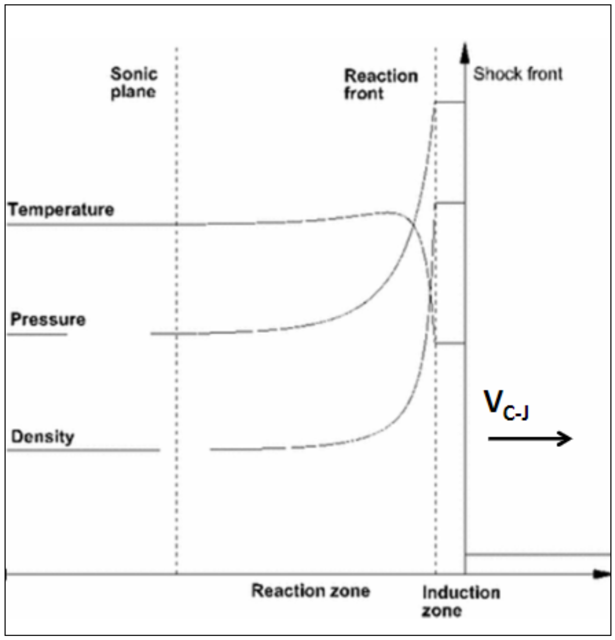

Figure 3: ZND detonation

2.4 Real detonation structure

The real detonation structure due to experiments may be:

2.4.1 Cellular detonation structure

That is the most common detonation structure

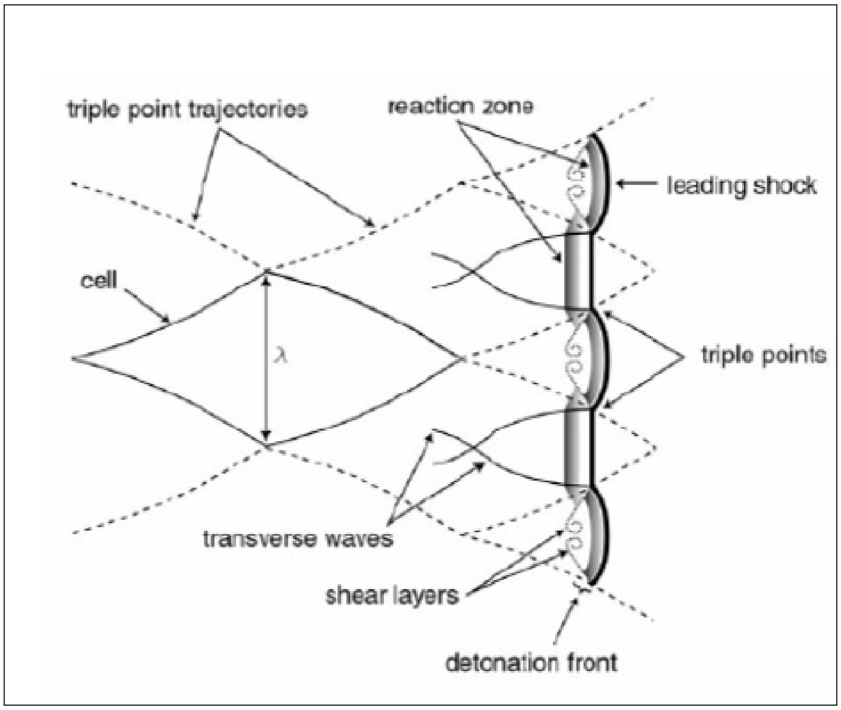

Figure 4: Cellular detonation

2.4.2 Rotating detonation structure

This structure is characteristic for parameters next to the detonation limits

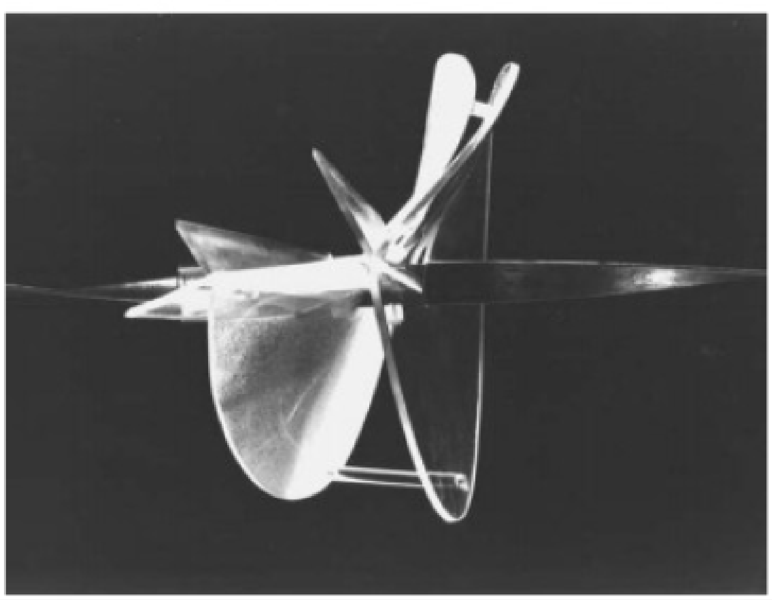

Figure 5: Rotating detonation

2.4.3 Zig-zag detonation structure

Zig-zag structure appears in rectangular pipes:

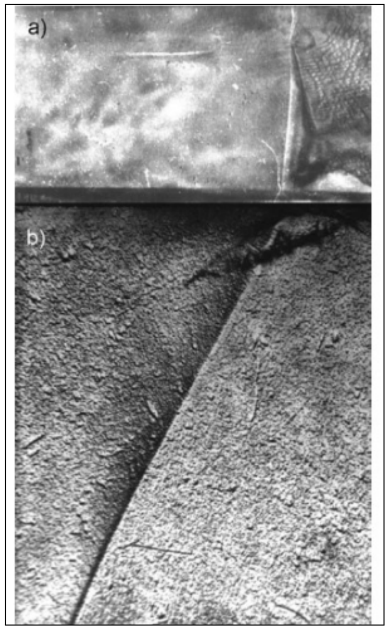

Figure 6: Zig-zag detonation

3 Model description

Detonation models were implemented using Cantera software. All of the assumptions are stated according to these models as well.
Initial parameters were changed and the C-J wave velocity was calculated for each combination. For thermodynamic and transport properties or the reaction rates GRI - 3.0 mechanism was used (a chemical mechanism developed by the Gas Research Institute to model natural gas combustion, including full NOx chemistry, a compilation of 325 reactions involving 53 species).

4 Results

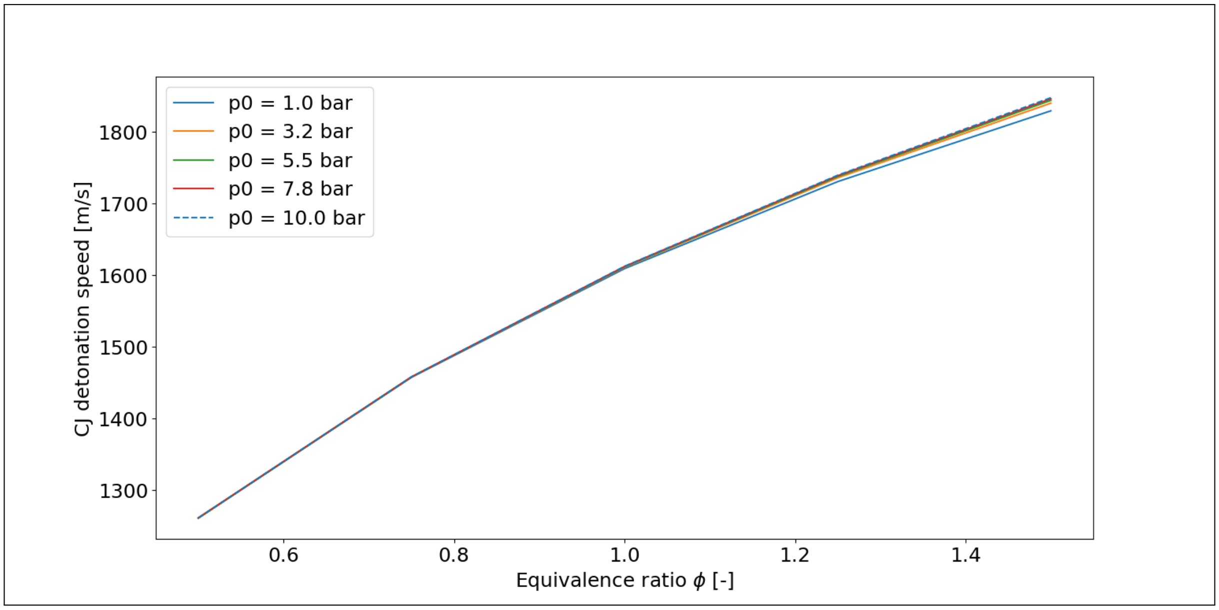

Figure 7: Relation of C-J speed and equivalence ratio ϕ for different initial pressure, const temperature

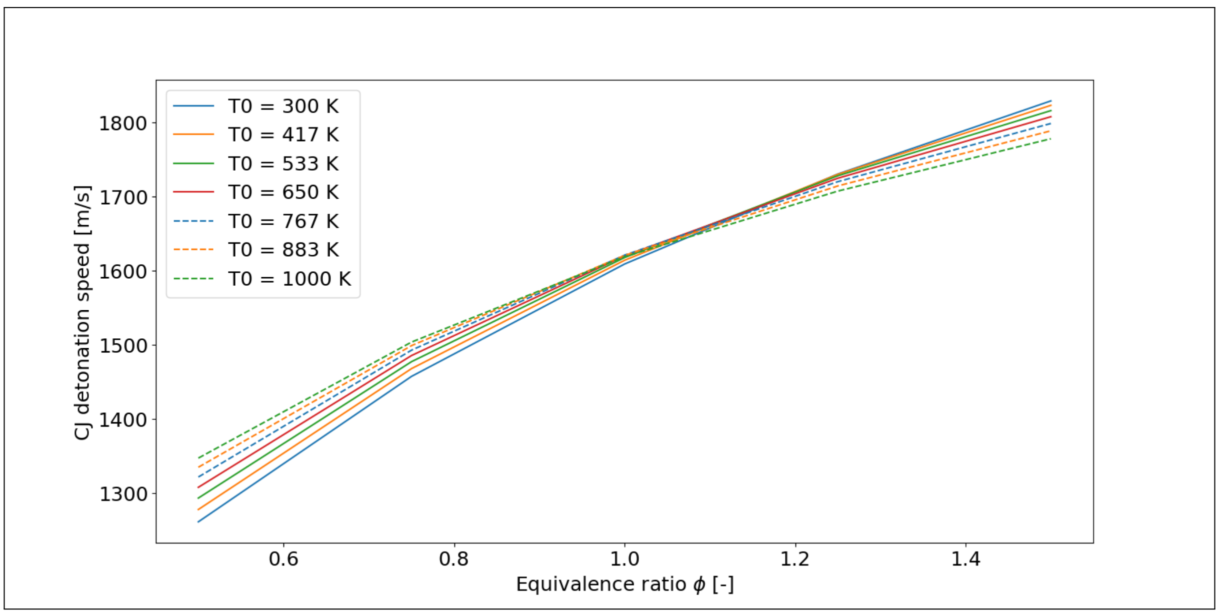

Figure 8: Relation of C-J speed and equivalence ratio ϕ for different initial temperature, const pressure

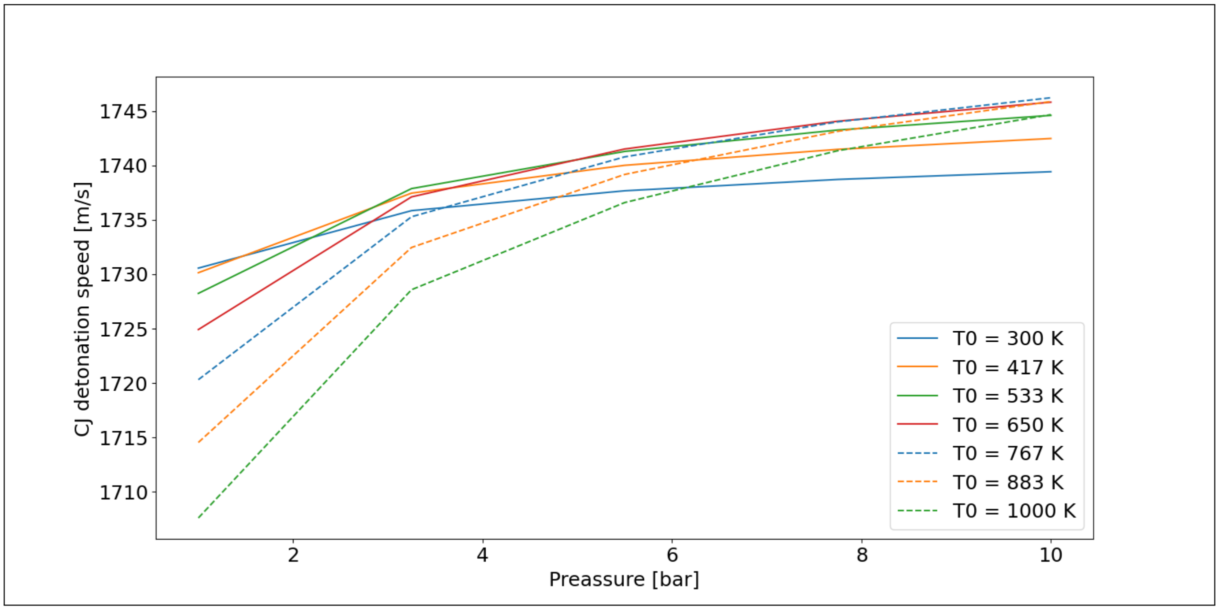

Figure 9: Relation of C-J speed and pressure for different initial temperature, const ϕ

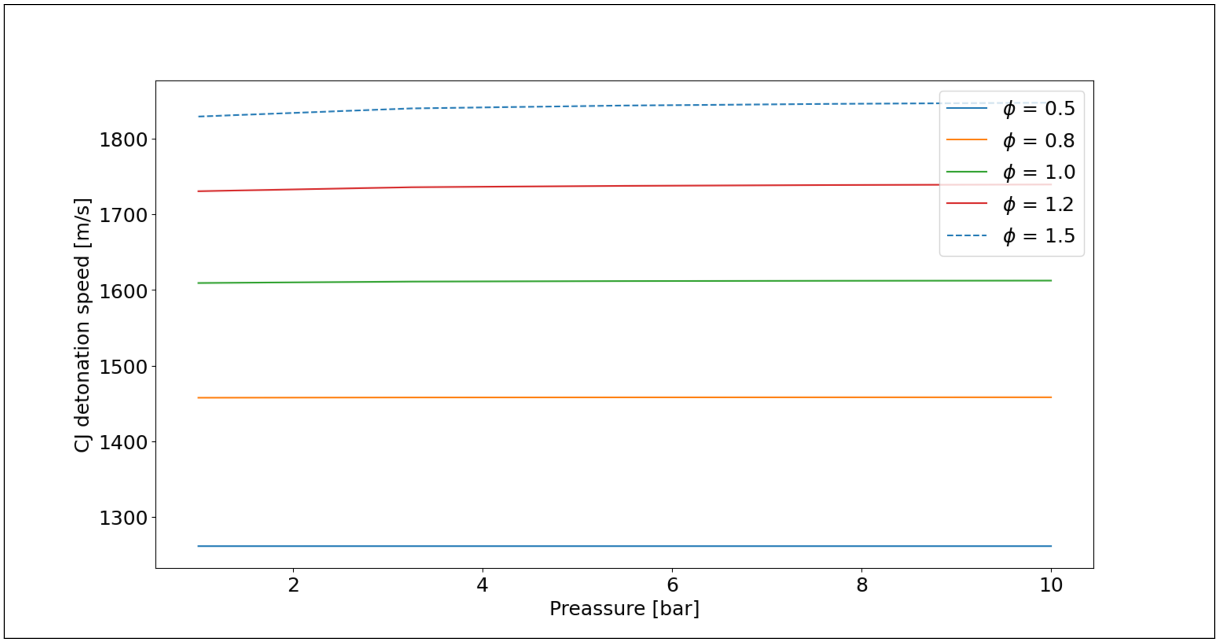

Figure 10: Relation of C-J speed and pressure for different initial ϕ, const temperature

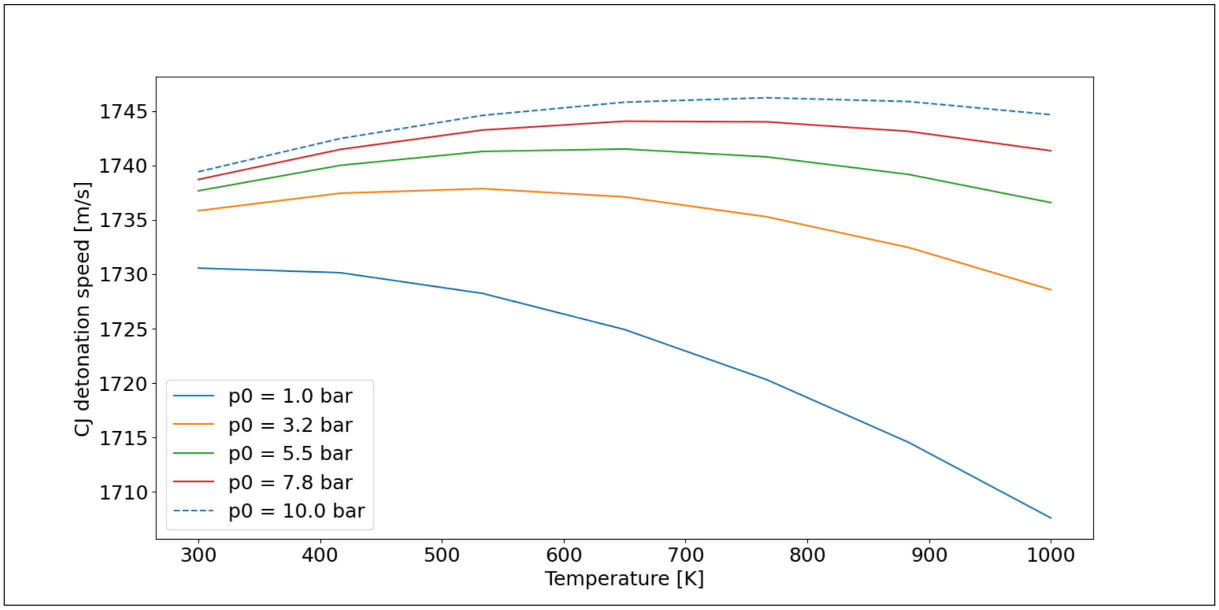

Figure 11: Relation of C-J speed and temperature for different initial pressure, const ϕ

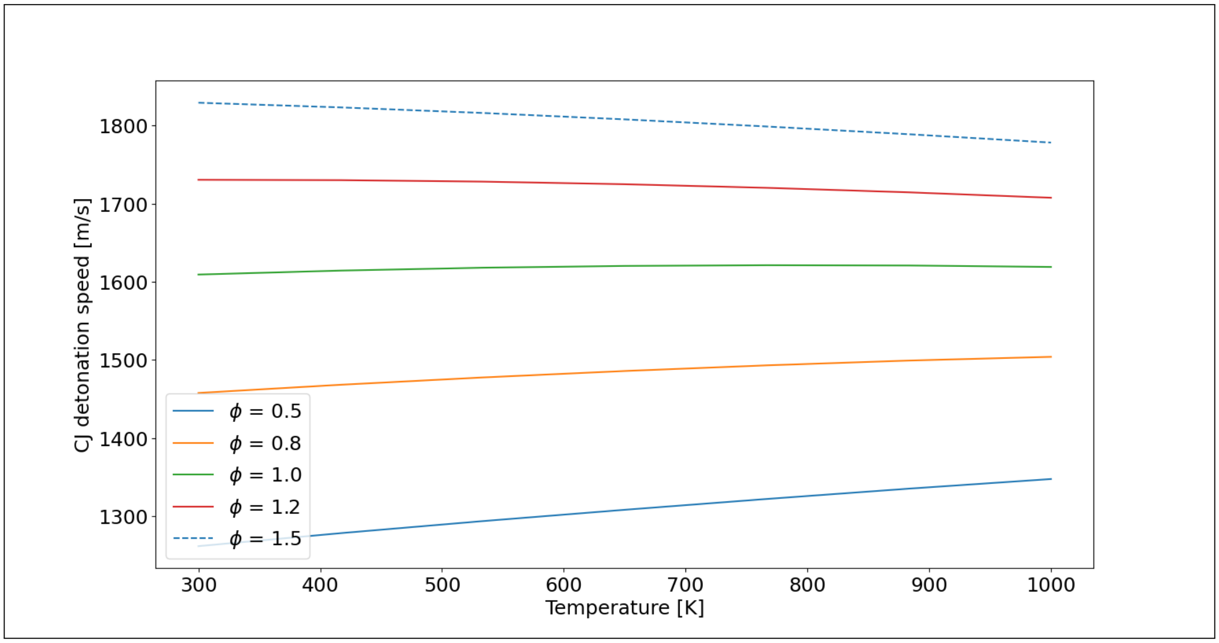

Figure 12: Relation of C-J speed and temperature for different initial ϕ, const pressure

5 Conclusions

- CJ speed (ϕ) for different initial pressure almost doesn't differ, for rising temperature, the curve is more horizontal. (figures 7,8)
- In Figure 9 it is seen that the CJ speed increases with rising pressure and has lower values for higher initial temperatures. CJ speed (pressure) graph is almost flat, detonation speed increases with ϕ. (Fig 10)
- According to Figure 11 the highest detonation speed is for initial temperature 800K, for the highest initial pressure. In the Figure 12 lines are almost flat - detonation speed almost does not depend on initial temperature for established ϕ.

6 Appendix

1. mkws.py

7 Bibliography

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3. 'Towards Detonation Theory' A. N. Dremin

4. $https://shepherd.caltech.edu/EDL/PublicResources/sdt/cti_mech.html$

5. https://github.com/Bazyl29/MKWS