

Warsaw University of Technology  
Faculty of Power and Aeronautical Engineering

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

Computer Methods in Combustion

author:  
**Jakub Kappes (313749)**

supervisor:  
**dr inż. Mateusz Żbikowski**

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# 1 Introduction

Detonation is a type of combustion where shock wave and flame front are bonded together. The reaction is of course exothermic. The flame front is propagating supersonically in the air-fuel mixture with speeds reaching 2 km/s and temperatures approaching 5300 deg.C.

In these project we are considering one-dimensional steady state Chapman-Jouguet (CJ) shock wave which is ideal and the simplest model. Chapman-Jouguet detonation is also the only stable type of detonation, so it is quite good approximation of any realistic process.

## 2 Theoretical background

### 2.1 Rankine-Hugoniot equations

To the volume in front of and behind the shock wave three conservation laws can be applied.

Conservation of mass:

$$\dot{m} = \rho_1(u_1 - U) = \rho_2(u_2 - U) \quad (1)$$

Conservation of momentum:

$$P_1 + \rho_1 u_1(u_1 - U) = P_2 + \rho_2 u_2(u_2 - U) \quad (2)$$

And conservation of energy:

$$\frac{1}{2}(u_1 - U)^2 + \frac{\kappa}{\kappa - 1} \frac{P_1}{\rho_1} = \frac{1}{2}(u_2 - U)^2 + \frac{\kappa}{\kappa - 1} \frac{P_2}{\rho_2} + H_p \quad (3)$$

where  $H_p$  is heat released in a portion of gas as a result of combustion. From mass and momentum equations the following formula can be obtained:

$$\frac{P_2 - P_1}{\frac{1}{\rho_1} - \frac{1}{\rho_2}} = \dot{m}^2 > 0 \quad (4)$$

From this formula follows the important fact that in a shock wave pressure and density changes can only be of the same sign (positive or negative). That is why we differentiate two kinds of combustion:

**detonative** - which causes pressure and density increase

**deflagrative** - which causes pressure and density decrease Transforming above-mentioned conservation equations we obtain Rankin'e-Hugoniot curve equation:

$$P\left(\frac{1}{\rho} \frac{\kappa + 1}{\kappa - 1} - \frac{1}{\rho_1}\right) - P_1\left(\frac{1}{\rho_1} \frac{\kappa + 1}{\kappa - 1} - \frac{1}{\rho}\right) - 2H_P = 0 \quad (5)$$

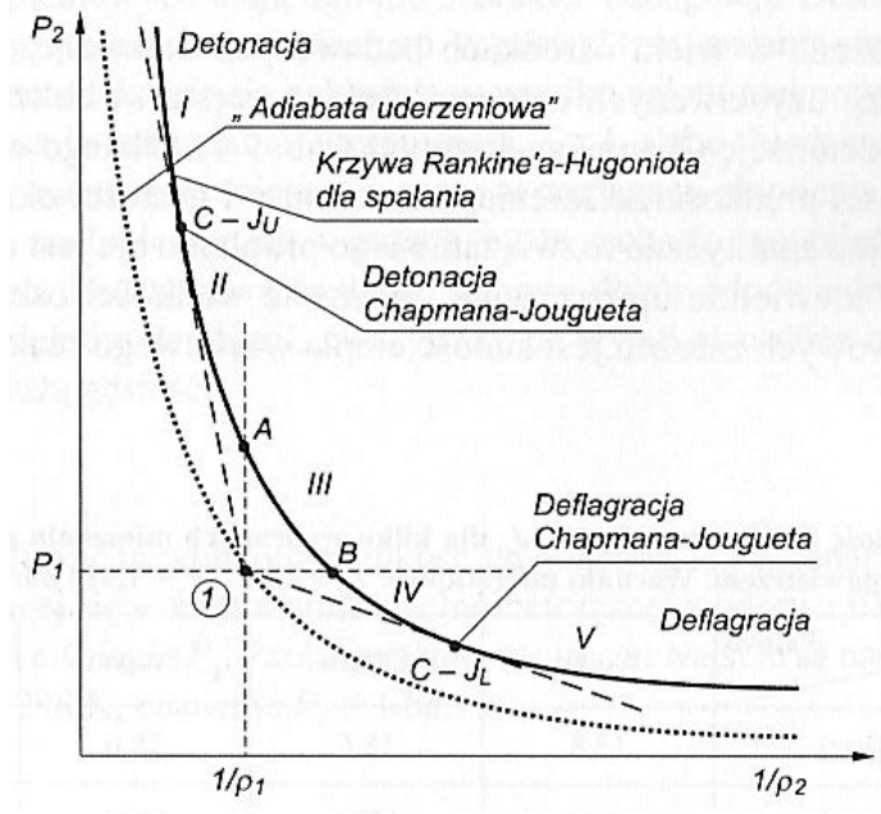


Figure 1: Rankine-Hugoniot curve for shock wave and combustion

The dotted line marks R-H curve for adiabatic shock wave, continuous line is moved upwards and marks R-H curve for combustion.

Section between points A and B has no physical meaning, section A-CJu represents weak detonation and Above CJu point - strong detonation. Analogically section from B to C-Jl stands for weak deflagration and beyond C-Jl point - strong deflagration.

Tangent line conducted from initial conditions to R-H curve marks parameters of Chapman-Jouguet detonation in the point of contact.

## 2.2 Chapman-Jouguet detonation

C-J wave moves forward with velocity that is supersonic in relation to preceding unburned mixture, but subsonic relative to burned fumes behind the shock. In reference frame bounded to the wave its propagation velocity is described as follows:

$$D = \frac{\rho_2}{\rho_1} a_2 = \frac{\rho_2}{\rho_1} \sqrt{\kappa_2 R_2 T_2} \quad (6)$$

Where  $a_2$  is local speed of sound in area behind the wave. Despite full analytical solution of this problem is not possible, by making little simplifications we can obtain good approximation. That's enough to assume that reactants and products specific heat is constants and that  $\kappa_1 \approx \kappa_2$  and equation above can be formed this way:

$$D = \sqrt{2(\kappa_1^2 - 1)(H_p + C_{p1}T_1)} \quad (7)$$

By making further assumption that  $Q \gg c_{p1}T_1$  we may shorten that to the form below:

$$D = \sqrt{2(\kappa_1^2 - 1)H_p} \quad (8)$$

These simplifications are permissible to be applied to C-J speed equation, because real detonation processes usually deviate a little from C-J theory thus loss of computations accuracy is not significant. According to equation (8) C-J detonation speed is a physical constant and this is generally proven true by the experiments.

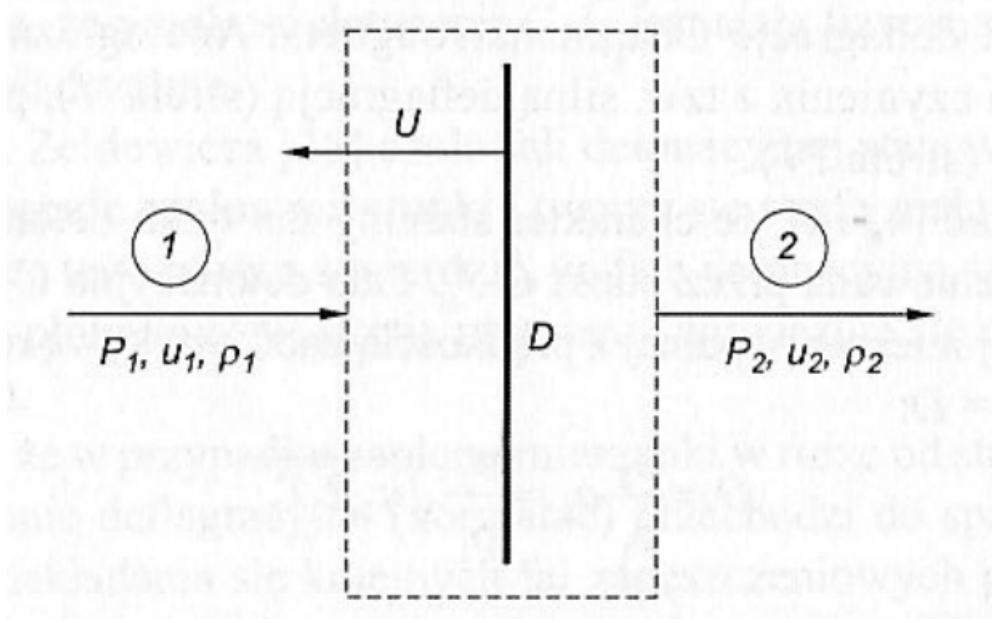


Figure 2: Gas parameters in the vicinity of Chapman-Jouguet detonation wave

### 2.3 Zeldovich-von Neumann-Döring detonation model

The ZND detonation model accounts a finite chemical reaction zone in contrast to C-J model where heat was released instantaneously as flame front passed.

As we can see on the figure below shock front adiabatically compresses reactants and then reaction starts, but needs some time to be fully conducted. That's why the temperature rises gradually.

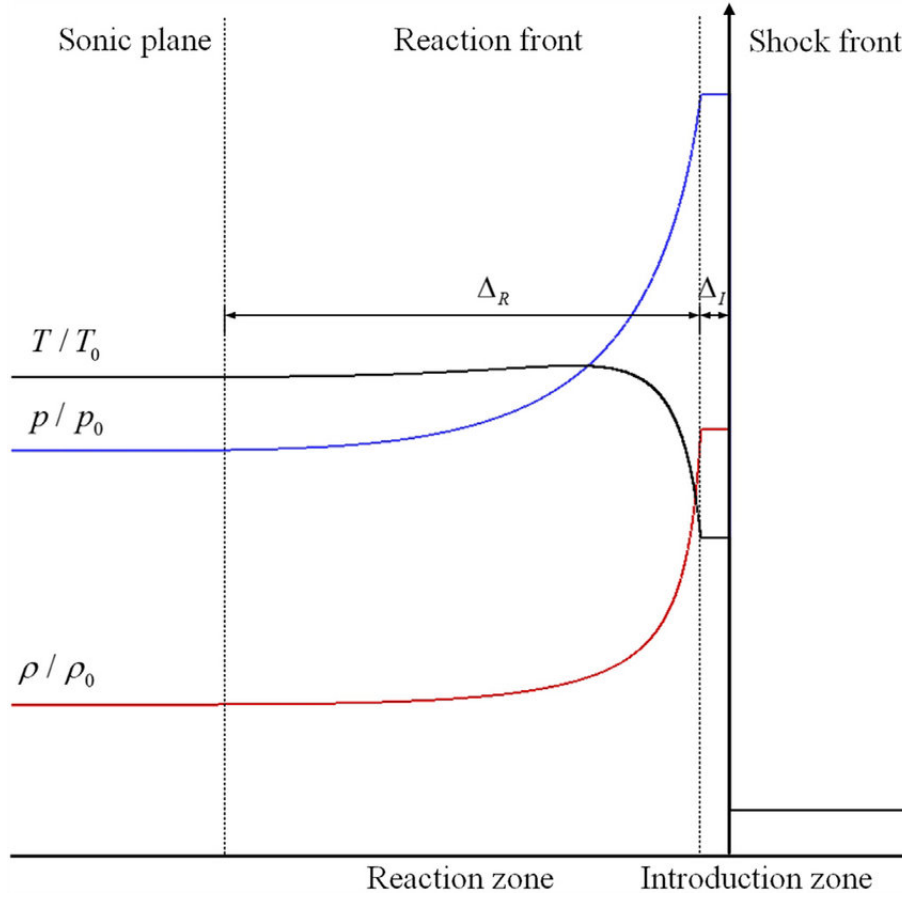


Figure 3: Gas parameters in the control volume around shock front

### 3 Model description

The results were obtained using Shock and Detonation Toolbox appended to Cantera environment. The program was written in Python3 and SD Toolbox's built-in function CJSpeed was used.

Realistic thermo-chemical mechanism of methane-air mixture combustion was described by GRI 3.0 mechanism (mechanism developed by Gas Research Institute, Caltech that takes into account 325 subreactions and 53 reactants including full NOx mechanisms that exist in methane combustion).

CJSpeed function was executed in a loop with three independent variables of initial temperature ranging from 300 K to 1000 K, initial pressure ranging from 1 bar to 10 bars and equivalence ratio ranging from 0.5 to 1.5.

## 4 Results

### 4.1 Constant equivalence ratio

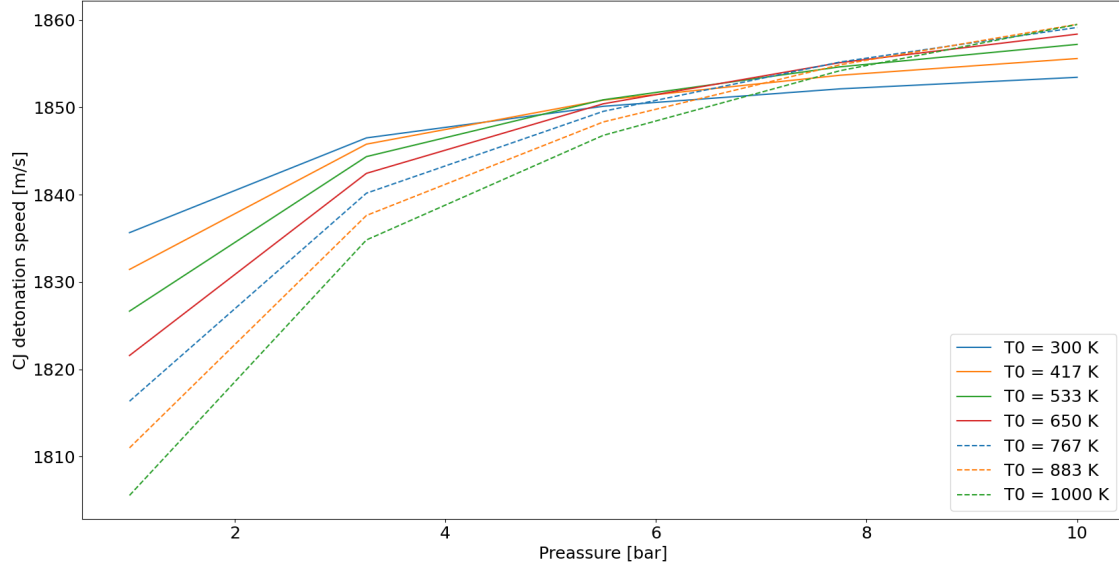


Figure 4: CJ-speed for various pressures at different temperatures,  $\phi = 1, 25$

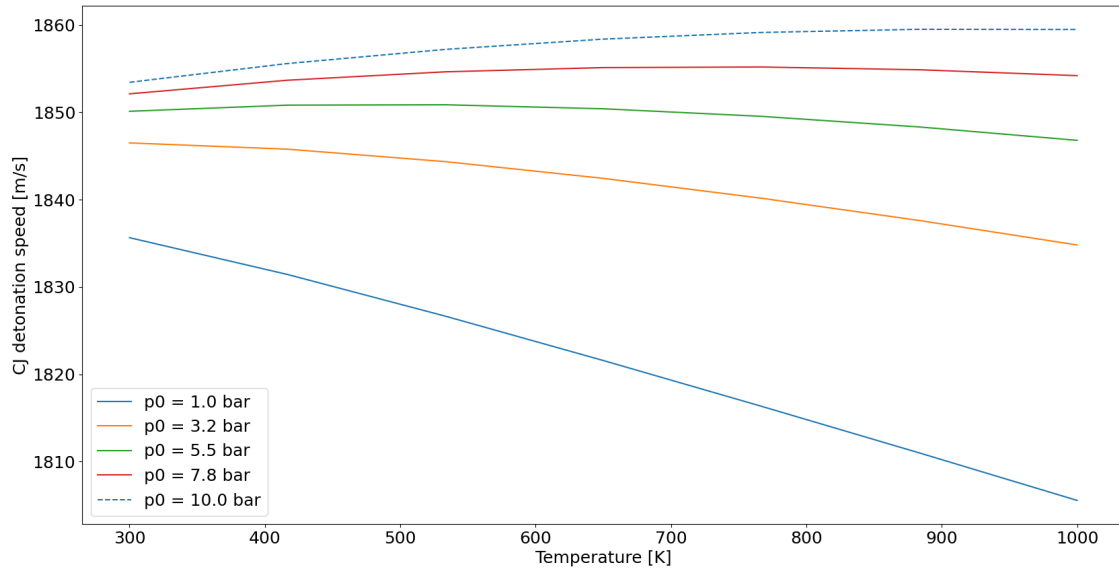


Figure 5: CJ-speed for various temperatures at different pressures,  $\phi = 1, 25$

## 4.2 Constant initial temperature

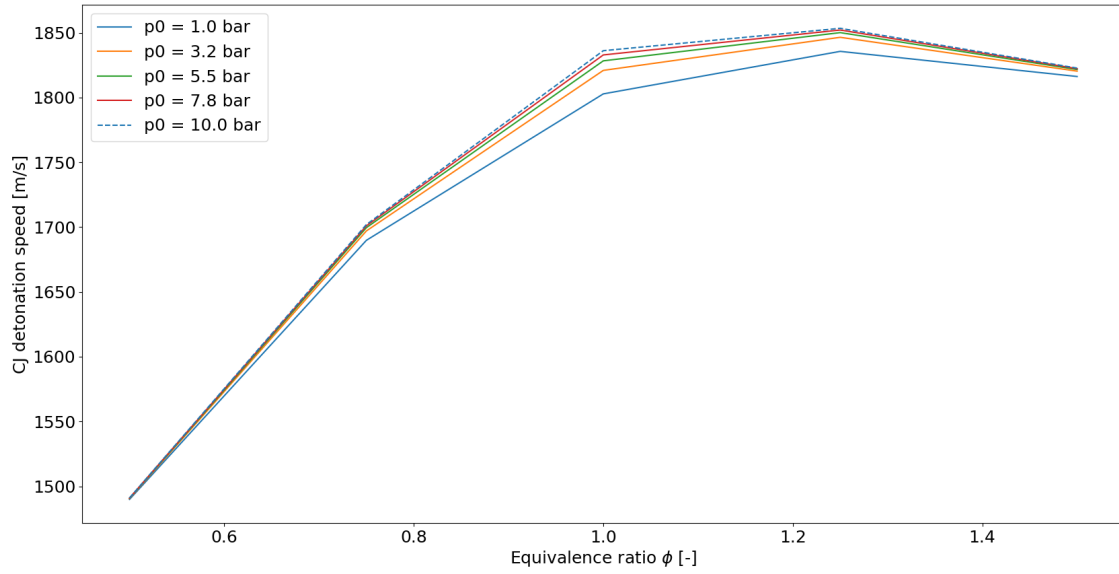


Figure 6: CJ-speed for various equivalence ratios at different pressures,  $T=300$  K

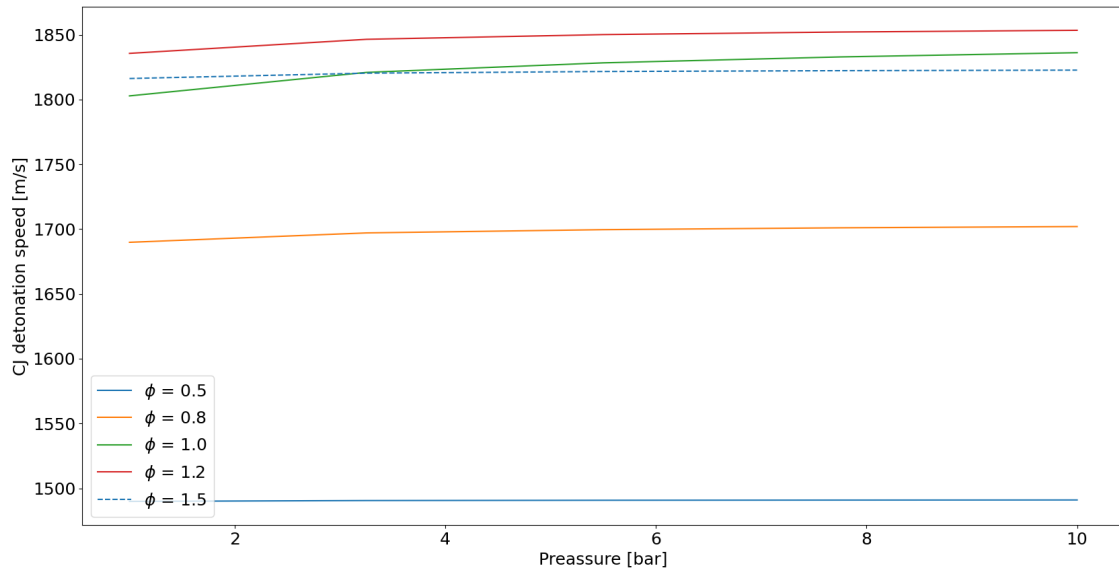


Figure 7: CJ-speed for various pressures at different equivalence ratios,  $T=300$  K



### 4.3 Constant initial pressure

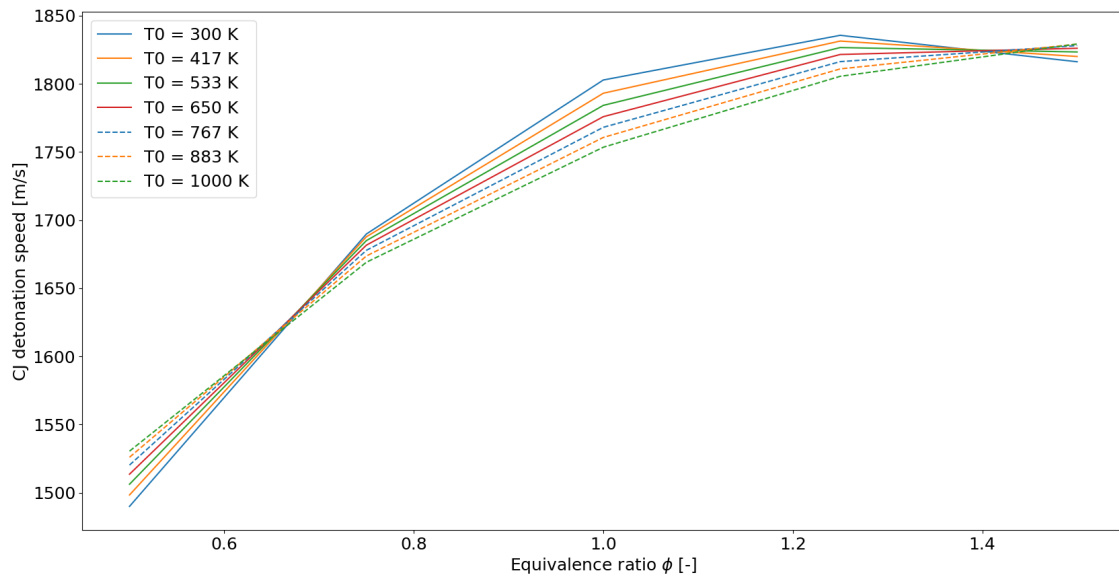


Figure 8: CJ-speed for various equivalence ratios at different temperatures,  $T=300$  K

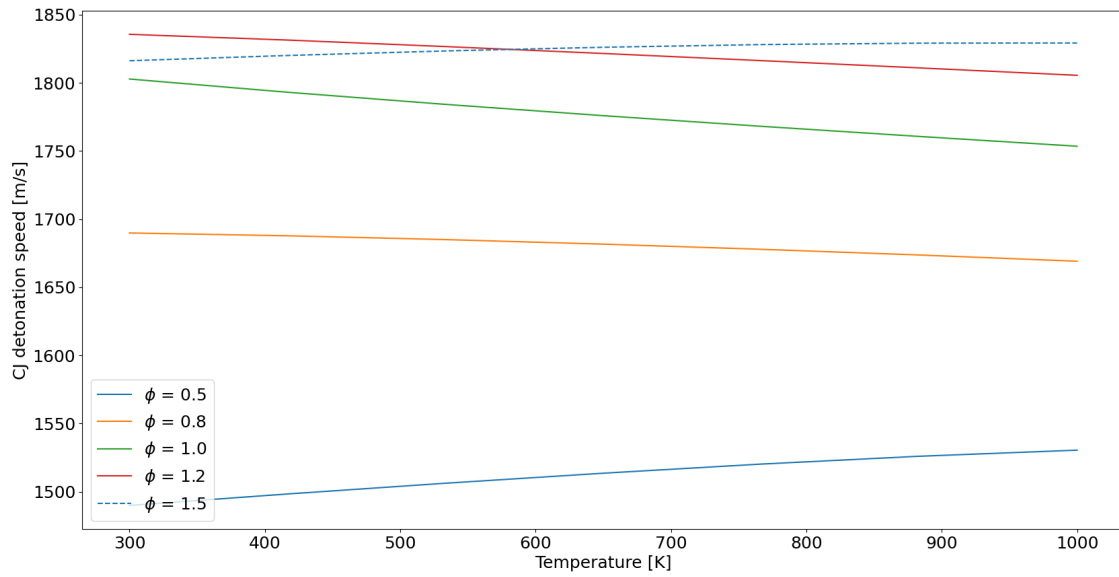


Figure 9: CJ-speed for various pressures at different equivalence ratios,  $T=300$  K

## 5 Conclusions

### 5.1 Constant equivalence ratio

CJ speed increases with pressure and the change mostly affects detonations with highest initial temperature.

Detonation has its optimal initial temperature for a given pressure where CJ speed is the highest. That optimal temperature rises as pressure increase.

### 5.2 Constant initial temperature

There is an optimal equivalence ratio which is universal for any initial pressure and equals ca. 1,2. These value may be caused by higher chemical efficiency for excess of oxidizer.

CJ speed does not depend on initial pressure and is constant for a given equivalence ratio.

### 5.3 Constant initial pressure

There is an optimal equivalence ratio where CJ speed is the highest, bu the optimum differs for various initial temperature. The higher initial temperature, the higher optimal equivalence ratio is.

For a given equivalence ratio CJ speed almost doesn't change with initial temperature.

## 6 Sources

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