

**WARSAW UNIVERSITY OF TECHNOLOGY**

**FACULTY OF POWER AND AERONAUTICAL ENGINEERING**

**COMPUTER METHODS IN COMBUSTION – PROJECT**

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**CALCULATION OF THE DETONATION VELOCITY IN A CONSTANT  
VOLUME FOR DIFFERENT MIXTURES**

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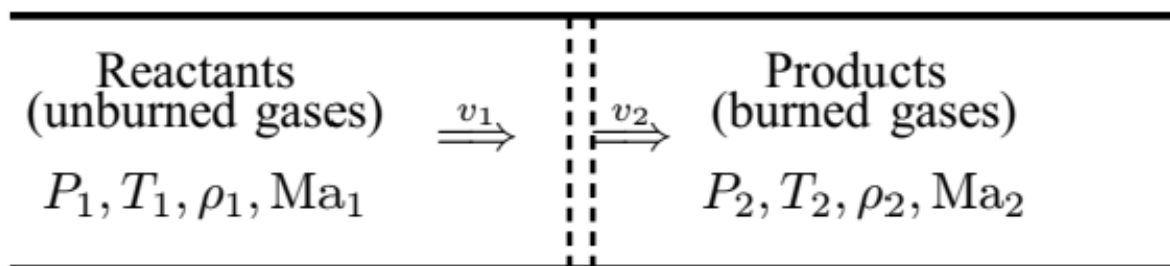
## 1 Introduction

The simplest theory to predict the behavior of detonation in gases is known as Chapman-Jouguet (CJ) theory developed around the turn of the 20<sup>th</sup> century. This theory describes detonation with a quite simple set of equations under a few assumptions as it models the whole process as a propagating shock wave accompanied by exothermic heat release. It does not concern an aspect of chemistry reaction or diffusive transport and reduces them to an infinitesimally thin layer. The following, more complex theory, was advanced during World War II independently by Zel'dovich, von Neumann and W. Deoring. It is called ZND theory and in a contrary to the previous one, provides details about the reaction zone of the detonation wave. According to this model, the energy release begins in a hot, shock-compressed material behind the shock front and continues until reaching thermodynamic equilibrium. In spite of the ZND theory's contribution, detonation velocity does not change in reference to CJ theory and remains as a pure thermodynamic function of temperature, pressure and mixture's composition. Although both theories are based on one-dimensional steady-state flow they define correct confines for possible solutions of multidimensional phenomenon. Moreover, calculated values of CJ velocity are comparable to mean detonation velocities measured during experiments, which proves that the models are well defined.

## 2 Theoretical background

### 2.1 Governing equations for a combustion wave in a premixed gas

Consider a straight conduit of constant cross section filled with mixture of combustible gases in which propagates a plane combustion wave along the axis. The process is considered in frame of the leading shock wave, so that a coordinate system is stationary to the wave.



**Figure 2.1.** One dimensional wave propagation inside the conduit.

Introduced model base on following assumption: one dimensional flow, constant cross section, ideal gas, constant specific heat capacity and adiabatic conditions. The set of equations describing presented flow consists of mass, momentum and energy conservation:

$$\begin{aligned}\rho_1 u_1 &= \rho_2 u_2 = \dot{m} \\ P_1 + \rho_1 u_1^2 &= P_2 + \rho_2 u_2^2 \\ h_1 + \frac{u_1^2}{2} &= h_2 + \frac{u_2^2}{2}\end{aligned}$$

where  $\dot{m}$  denotes a mass flux per area unit. An additional equation comes from ideal gas law:

$$p = \rho R T$$

where  $R$  stands for a specific gas constant (with index 1 or 2 for inlet and outlet gases respectively). Stagnation enthalpy represents the sum of enthalpy of formation and free enthalpy:

$$h(T) = \sum Y_i h_{f_i}^0 + \sum Y_i \int_{T_0}^T c_{p_i} dT = \sum Y_i h_{f_i}^0 + c_p (T - T_0)$$

for constant specific heat capacity.

Substituting for enthalpy in energy conservation equation:

$$\begin{aligned}c_p T_1 + \frac{u_1^2}{2} + \left( \sum Y_i h_{f_i}^0 \right)_1 - \left( \sum Y_i h_{f_i}^0 \right)_2 &= c_p T_2 + \frac{u_2^2}{2} \\ c_p T_1 + \frac{u_1^2}{2} + q &= c_p T_2 + \frac{u_2^2}{2}\end{aligned}$$

where  $q$  denoted heat released.

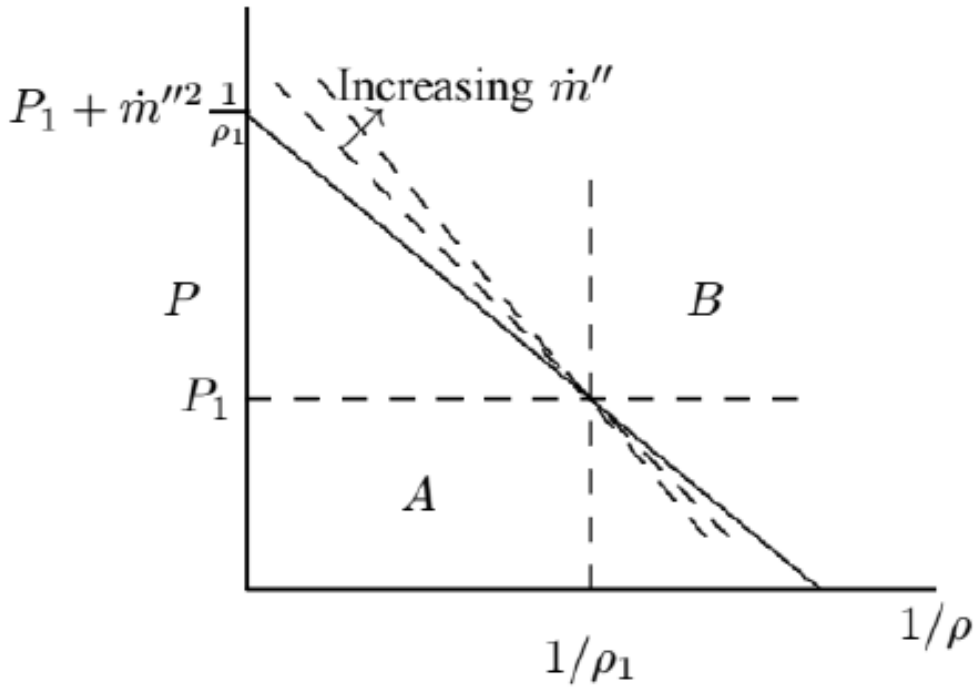
Foregoing formulas leave five unknowns and four equations. However, when only equations for mass and momentum conservation are taken into account and merged together it results with a relation between pressure and density in front of and behind the wave as a function of the mass flux.

$$\frac{P_2 - P_1}{\frac{1}{\rho_2} - \frac{1}{\rho_1}} = -\dot{m}^2$$

By plotting pressure  $P$  with respect to density  $\rho$  for the given value of mass flux  $\dot{m}$ , **Rayleigh lines** are obtained. For given  $P_1$  and  $\rho_1$ :

$$P = a \left( \frac{1}{\rho} \right) + b$$

$$a = -\dot{m}^2 \quad b = P_1 + \dot{m}^2 \left( \frac{1}{\rho_1} \right)$$



**Figure 2.2.** Rayleigh lines in  $\left( \frac{1}{\rho}, P \right)$  coordinates.

Thus, a great deal of insight is gained by observing the results. The slope of each and every Rayleigh line is always negative due to  $a = -\dot{m}^2$  so they can only exist outside the regions A and B on Figure 2. It brings to a conclusion that the physics of detonation only allows processes which leads to either increase in both pressure and density or to decrease at the same time.

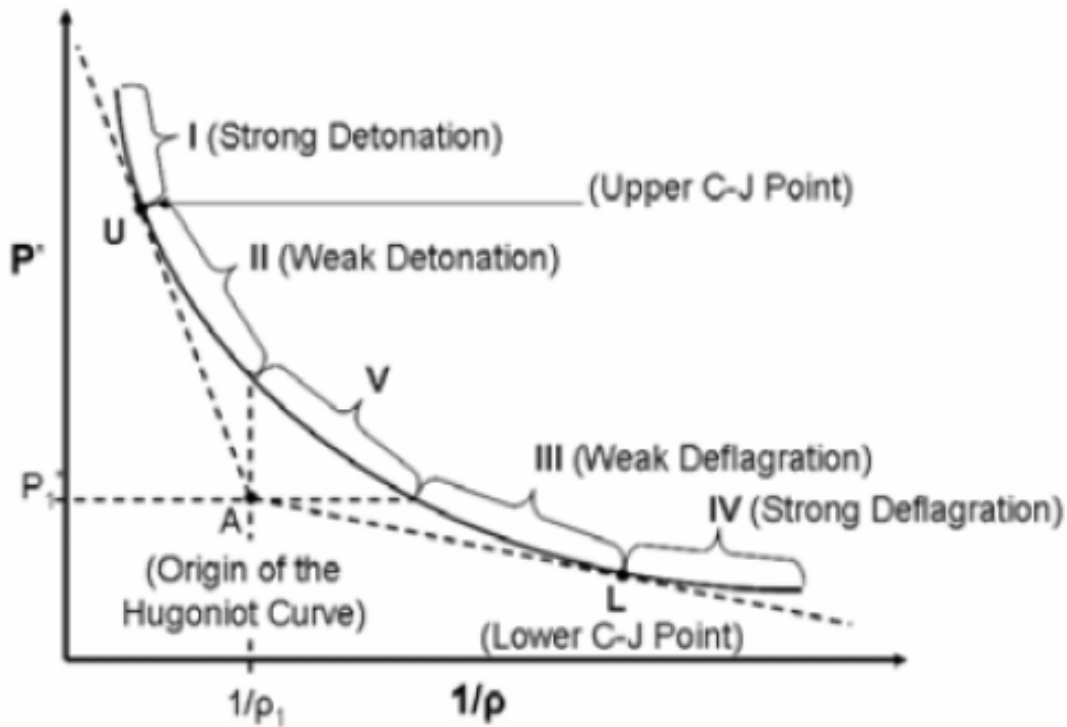
By taking conservation of energy into consideration the following equation comes up:

$$\frac{\kappa}{\kappa - 1} \left( \frac{P_2}{\rho_2} - \frac{P_1}{\rho_1} \right) - \frac{1}{2} \left( \frac{1}{\rho_1} + \frac{1}{\rho_2} \right) (P_2 - P_1) - q = 0$$

It is called the **Rankine-Hugoniot relation**. For the heat release being equal to zero ( $q = 0$ ), this equation is referred to as the Hugoniot relation for a shock.

## 2.2 Observation of Rankine-Hugoniot curve

Rankine-Hugoniot (R-H) curve is a set of solutions – states after combustion, connected to the initial conditions  $\left(\frac{1}{\rho_1}, P_1\right)$  by the Rankine-Hugoniot relation. Drawing it together with four Rayleigh lines in the same diagram leads to creation of five different regions along the curve.



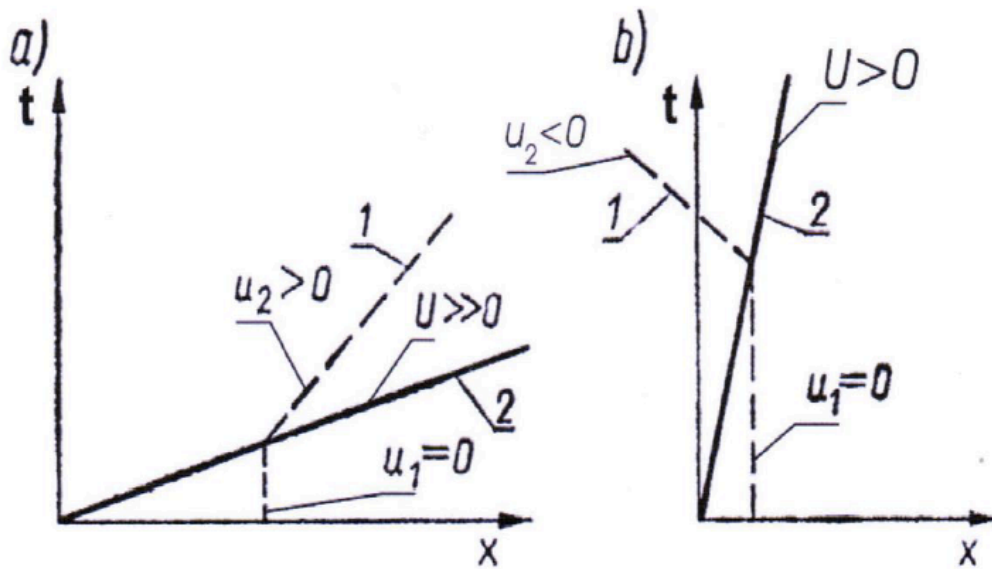
**Figure 2.3.** Rankine-Hugoniot curve.

Region V lays in a forbidden area to Rayleigh lines, thus solutions located within it are not physically realizable for the reason introduced in the previous section. Processes which result in decrease of pressure and density are called deflagration, and those leading to increase of initial parameters are called detonation. Detonation at the upper C-J point is the only one detonation which is stable. Its speed in regard of combustion gases is sonic and is the smallest value of detonation speed (the bigger slope of Rayleigh line, the greater speed).

Recalling mass and momentum conservation equations enables determining direction in which combustion gases propagate. Transforming those equations brings the following formula:

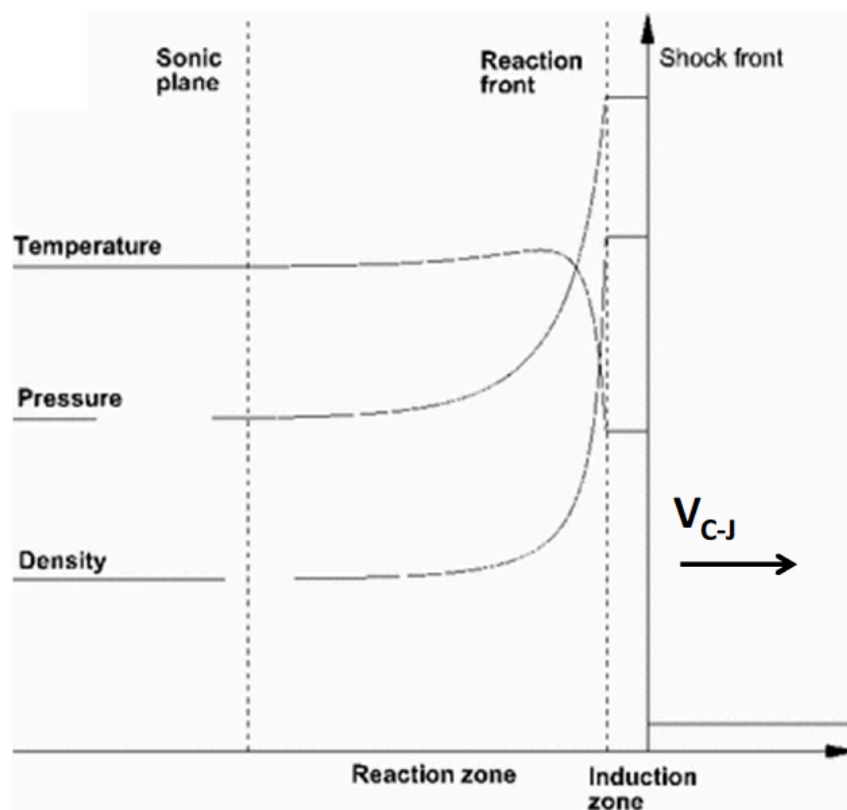
$$\dot{m} = \frac{P_2 - P_1}{u_1 - u_2} > 0$$

One can prove that in case of detonation, combustion gases travel in the same direction as shock wave and during deflagration – the other way.



**Figure 2.4.** Combustion gases propagation in case of a) detonation b) deflagration, where 1-path of fluid element in time, 2-path of flame front in time.

### 2.3 Internal structure of a plane detonation. The ZND theory.

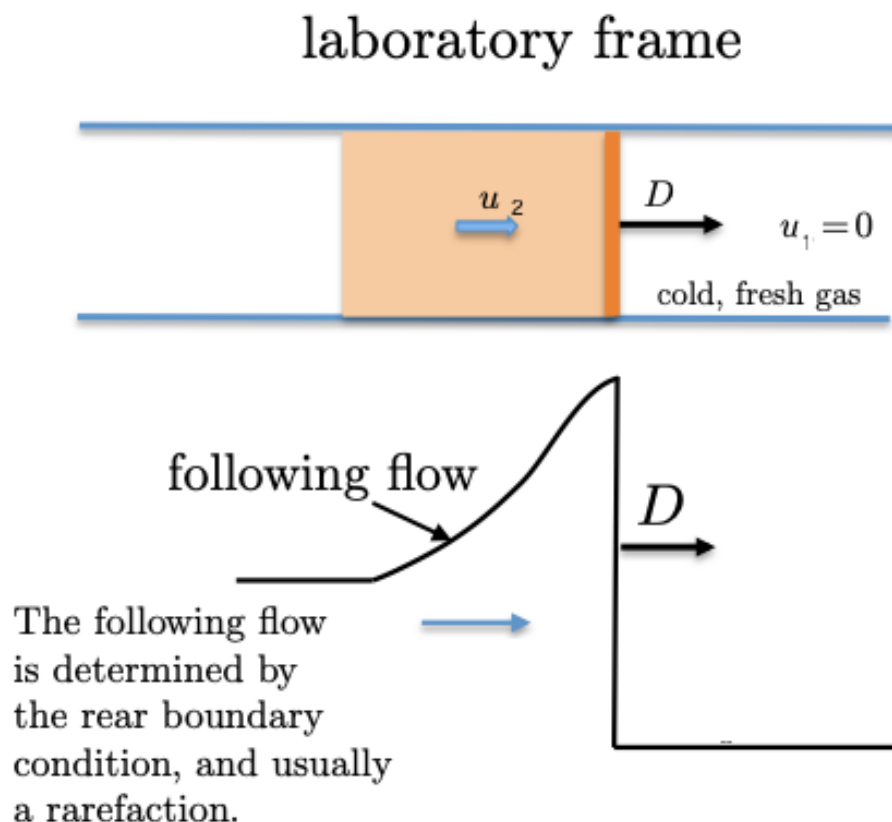


**Figure 2.5.** ZND theory.

Detonation wave consists of shock wave and flame front “glued” to it. This model admits finite-rate chemical reactions and thus describes a detonation as an infinitesimally thin shock wave followed by a zone of exothermic chemical reaction. With a reference frame of stationary shock, the following flow is subsonic, so that an acoustic reaction zone follows immediately behind the lead front. This kind of propagation is known as **Chapman-Jouguet condition**.

Ahead of the wave, the gas is quiescent and there is insignificant reaction. Passage through the lead shock the gas is compressed, the pressure increases tremendously, and its temperature rises thousands of degrees. The ensuing chemical reaction goes to completion very rapidly in a relatively thin reaction zone (or fire) behind the shock. Compression and therefore the significant increase in temperature drive the combustion processes and simultaneously the combustion processes sustain shock wave.

#### 2.4 Chapman-Jouguet detonation velocity calculation



**Figure 2.6.** Detonation wave in laboratory frame and related velocity change over passage.



Detonation velocity in reference to combustion gases behind the wave  $D_2 = D - u_2$  can be expressed by formula:

$$D_2 = \frac{1}{\rho} \sqrt{\frac{P - P_1}{\frac{1}{\rho_1} - \frac{1}{\rho}}}$$

which stems from conservation of momentum.

Rankine-Hugoniot curve's slope in upper C-J point is equal to:

$$\frac{dP}{d\frac{1}{\rho}} = -\frac{P - P_1}{\frac{1}{\rho_1} - \frac{1}{\rho}}$$

Using this information and substituting in equation for  $D_2$  gives:

$$D_2 = \frac{1}{\rho} \sqrt{\frac{dP}{d\frac{1}{\rho}}} = -\sqrt{\frac{dP}{d\rho}}$$

Because isentropic sound velocity equals:

$$a = \sqrt{\frac{dP}{d\rho}}$$

Hence  $D_2 = a_2$  which means that detonation velocity in regard of combustion gases is sonic and supersonic in regard of unburned mixture.

Assuming that  $Q \gg c_{v1}T_1$  and  $\kappa_1 \approx \kappa_2$  relations for C-J velocity comes up:

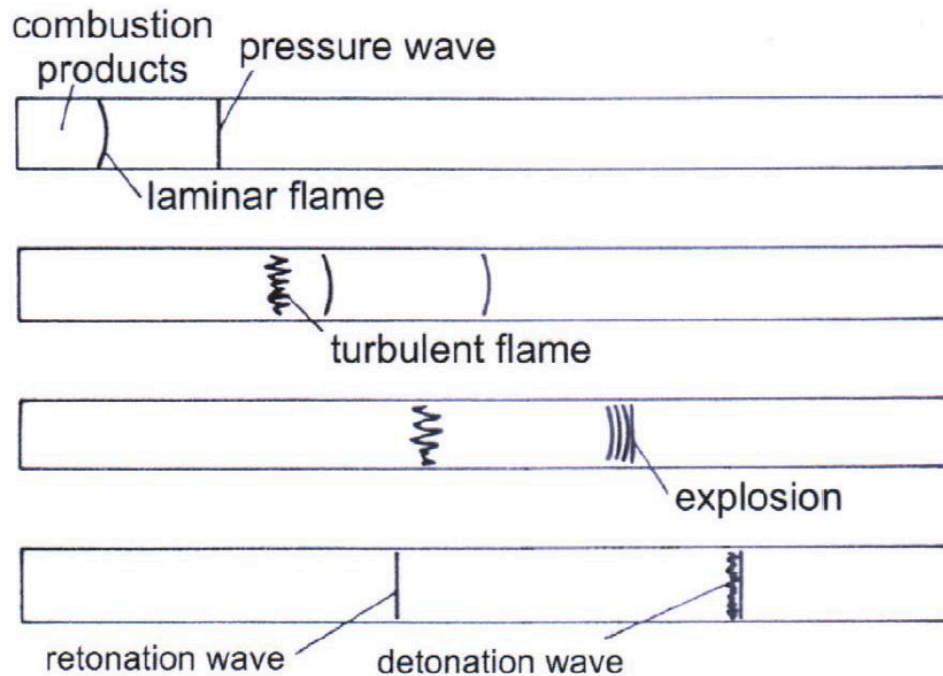
$$v_{C-J} = D_1 = \sqrt{2(\kappa_1^2 - 1)Q}$$

An important observation can be made that  $v_{C-J}$  is a constant physical value for a given gas mixture.

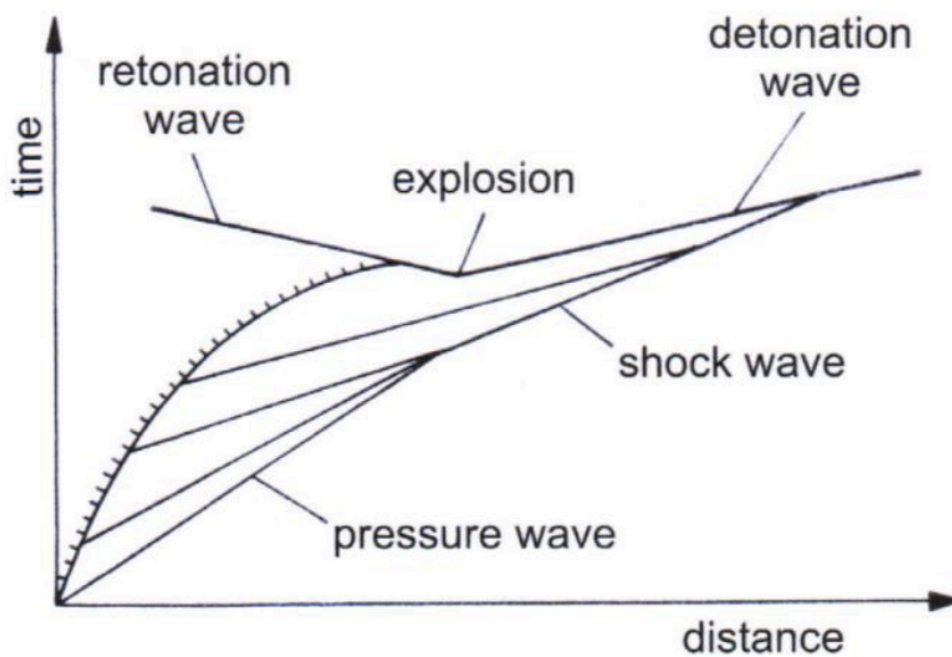
## 2.5 Deflagration to detonation transition (DDT)

Deflagration to detonation transition, often referred to as DDT, can be observed in a long conduit covered from one side. At first at rest, combustible mixture is ignited at the beginning of the conduit on covered side. Formation of a laminar flame occurs and so that process begins. Between the flame front and covered end combustion gases expand and rise the pressure. Due to inertia of “pushed” fresh mixture elementary pressure waves are formed in front of the flame front. These waves catch up to each other as every next one propagates in a hotter environment and lead to formation of a shock wave, which temperature is higher than the flashpoint of the

mixture. After a short delay ignition takes place and rapidly transform into a thermal explosion. It initiates creation of two waves propagating in opposite directions – detonation wave and retonation wave.



**Figure 2.7.** Step by step DDT in a long conduit.



**Figure 2.8.** Relation between distance and time for DDT.

### 3. Modeling method description

In order to obtain the computation results of detonation speed for analyzed mixtures in constant volume the Shock & Detonation Toolbox software is used. It is a collection of numerical routines that enables the solution of standard problems for gas-phase explosions using realistic thermochemistry and detailed chemical kinetics. The SD Toolbox employs Dave Goodwin's Cantera software for the chemistry functionality and uses either MATLAB or Python (and related libraries) for scripting. The Cantera package provides conversion utilities from legacy formats in order to make use of existing database of chemical kinetics and thermochemistry.

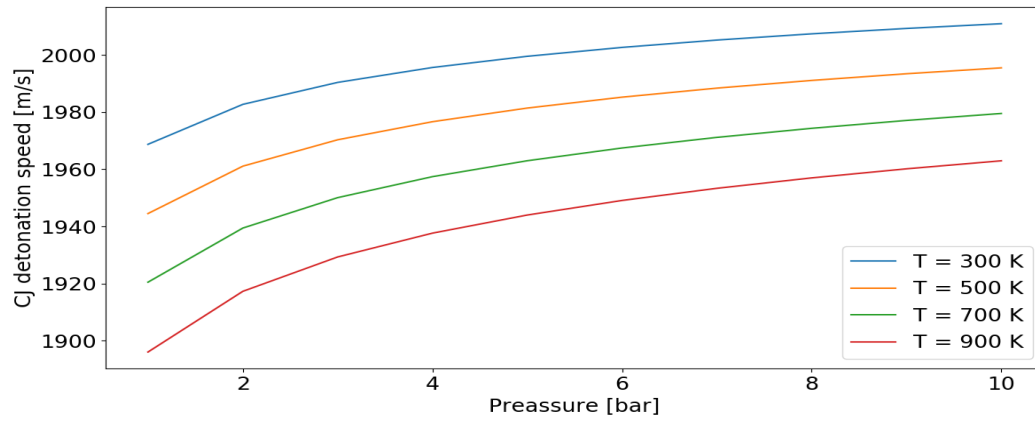
In the scope of this paper Python interface is used to apply numerical routine for the computation of CJ detonation speed.

Chosen data set used to model thermochemistry and reaction mechanism is GRI-Mech 3.0, which is an optimized mechanism designed to model natural gas combustion, including NO formation and reburn chemistry. This version covers 53 species, 325 reactions, temperatures in range from 300 to 5 000 K and also includes transport parameters.

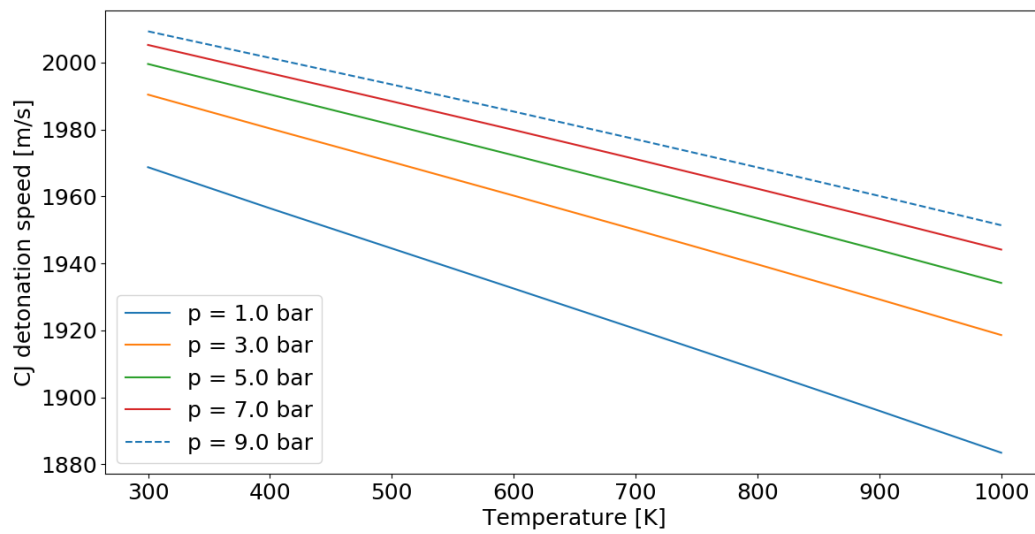
Computation is held in nested loops with varying initial conditions of pressure and temperature for nine mixtures created by mixing nine different species with air. All reactions are conducted under stoichiometric conditions.

## 4. Results

$H_2$ :

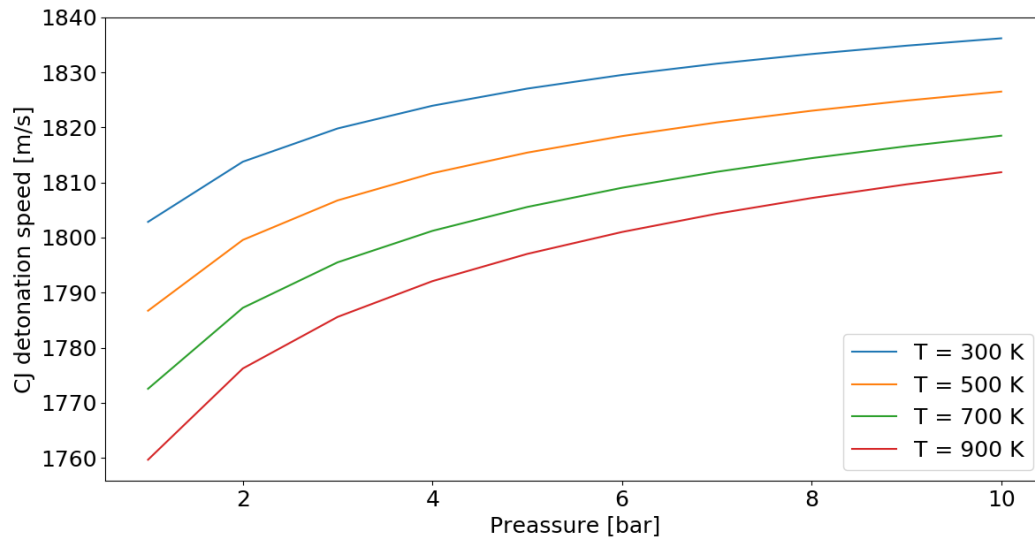


**Figure 4.1.** CJ detonation speed as function of pressure for different initial temperature

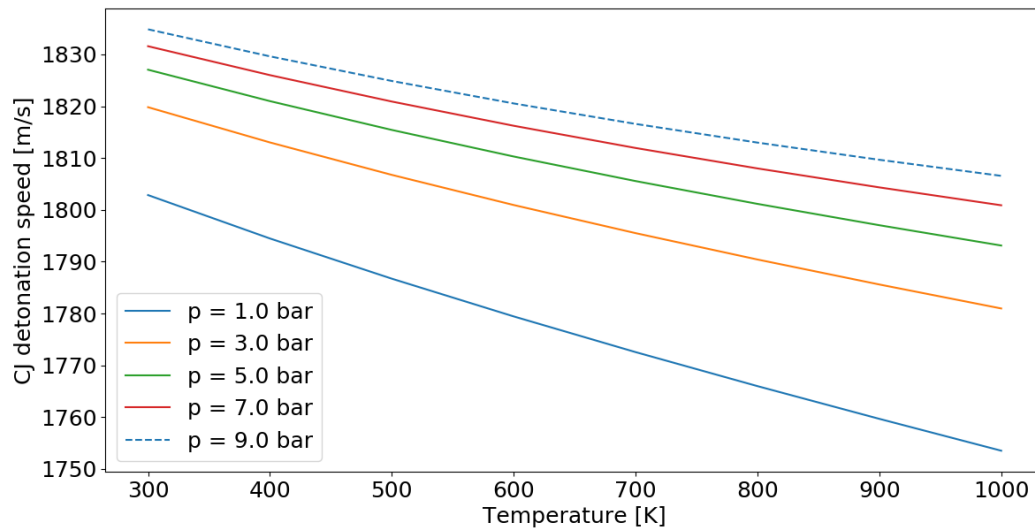


**Figure 4.2.** CJ detonation speed as function of temperature for different initial pressure

$CH_4$ :

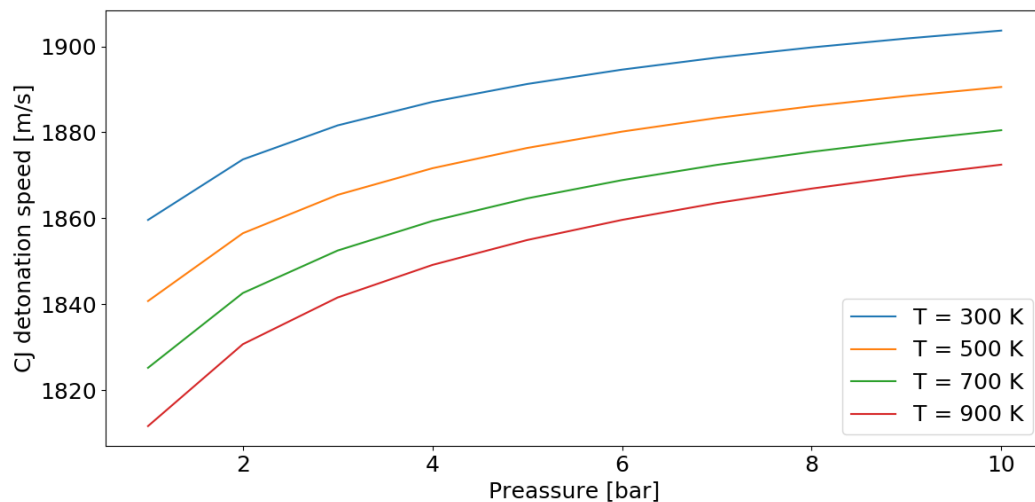


**Figure 4.3.** CJ detonation speed as function of pressure for different initial temperature

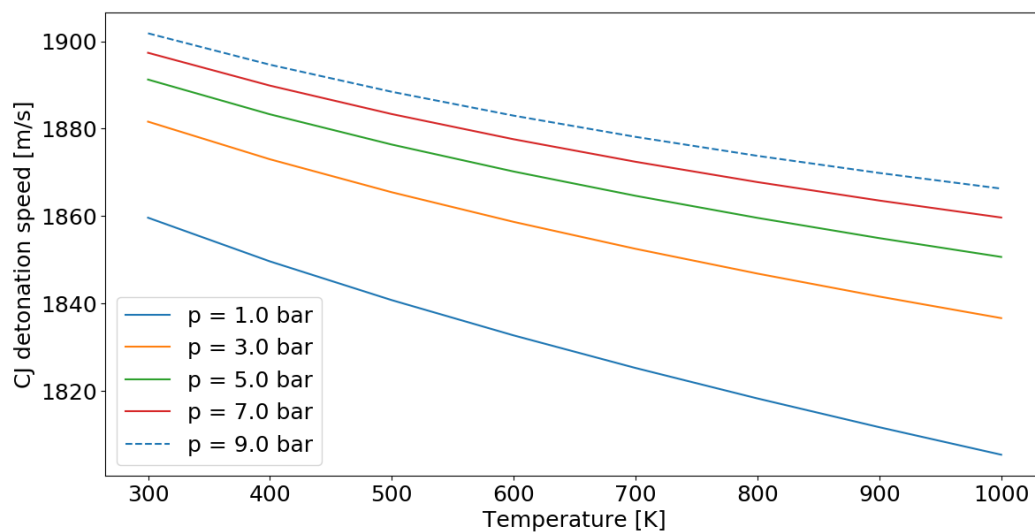


**Figure 4.4.** CJ detonation speed as function of temperature for different initial pressure

$C_2H_5$ :

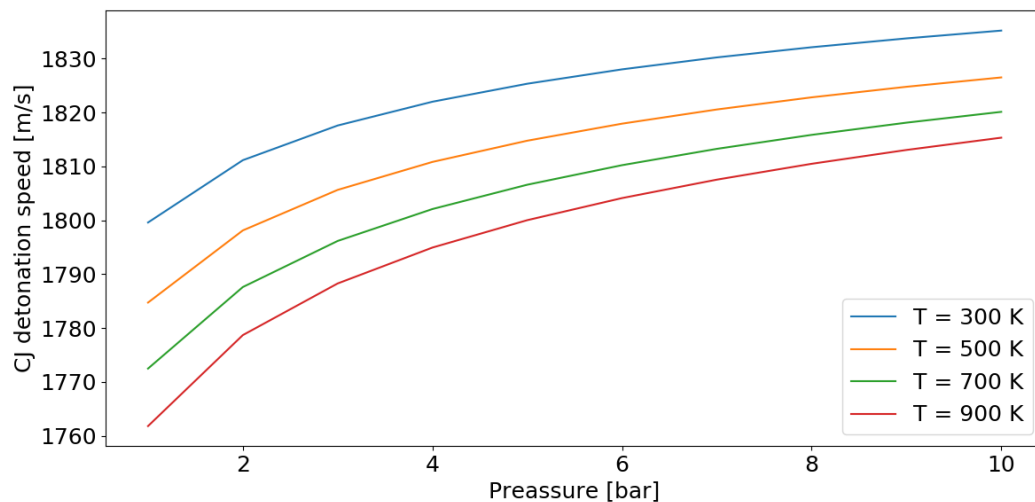


**Figure 4.5.** CJ detonation speed as function of pressure for different initial temperature

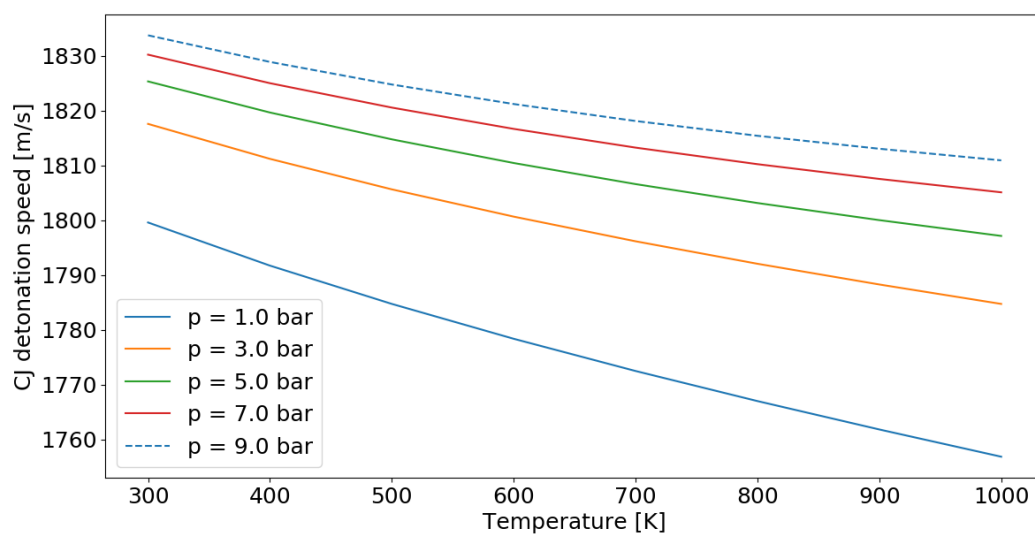


**Figure 4.6.** CJ detonation speed as function of temperature for different initial pressure

$C_3H_8$ :

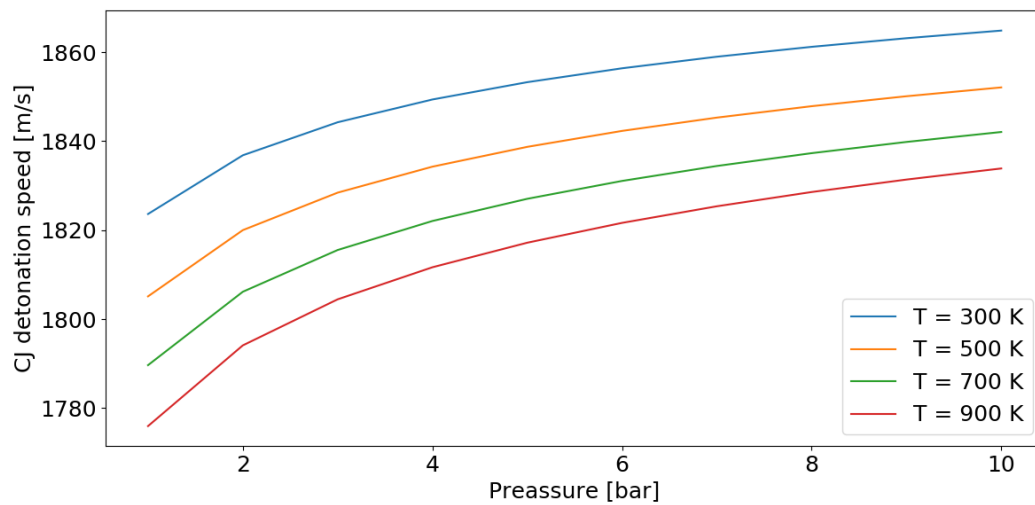


**Figure 4.7.** CJ detonation speed as function of pressure for different initial temperature

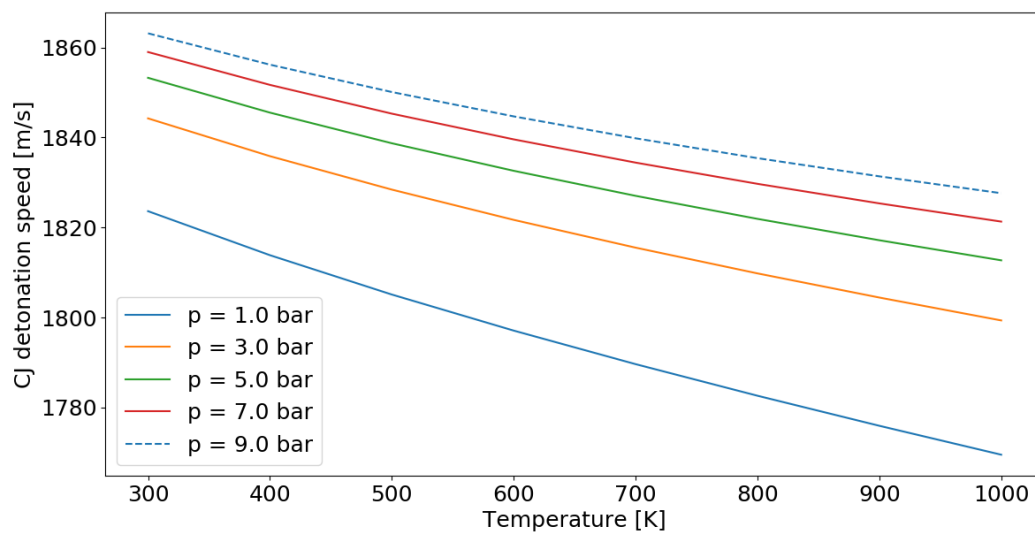


**Figure 4.8.** CJ detonation speed as function of temperature for different pressure

$C_2H_4$ :



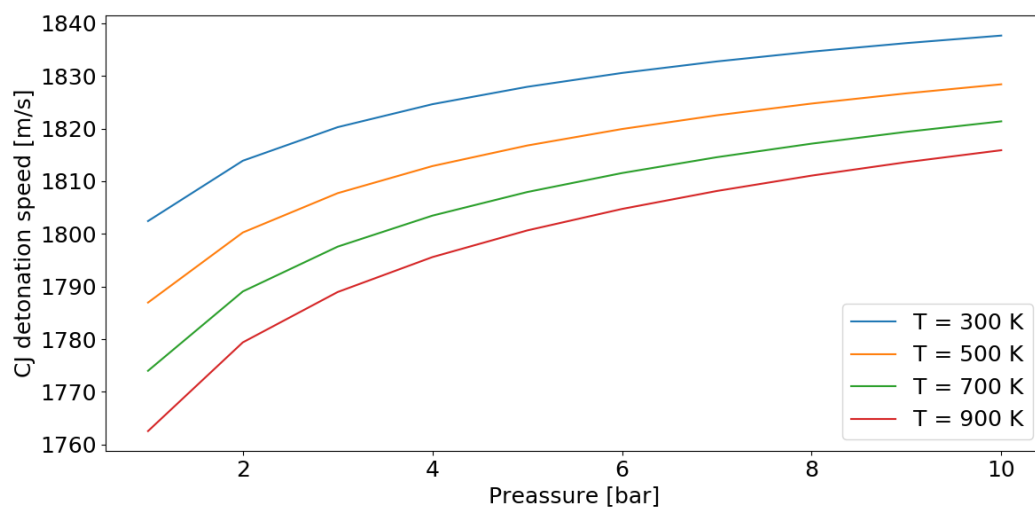
**Figure 4.9.** CJ detonation speed as function of pressure for different initial temperature



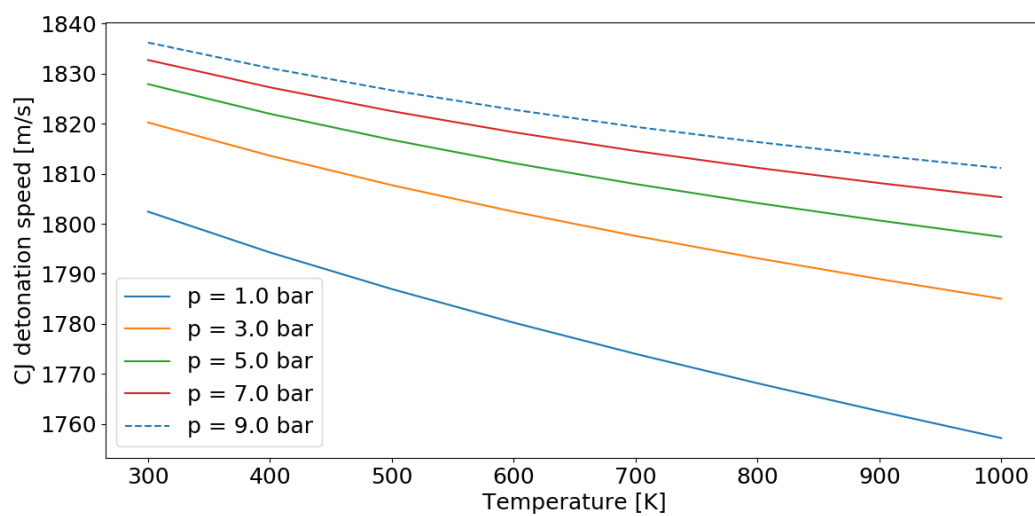
**Figure 4.10.** CJ detonation speed as function of temperature for different pressure



$C_2H_6$ :

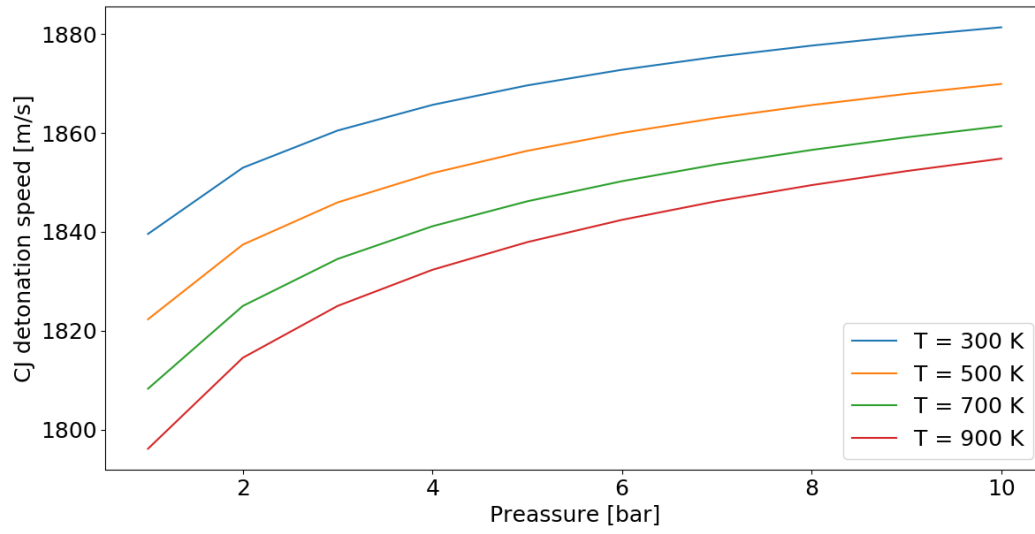


**Figure 4.11.** CJ detonation speed as function of pressure for different initial temperature

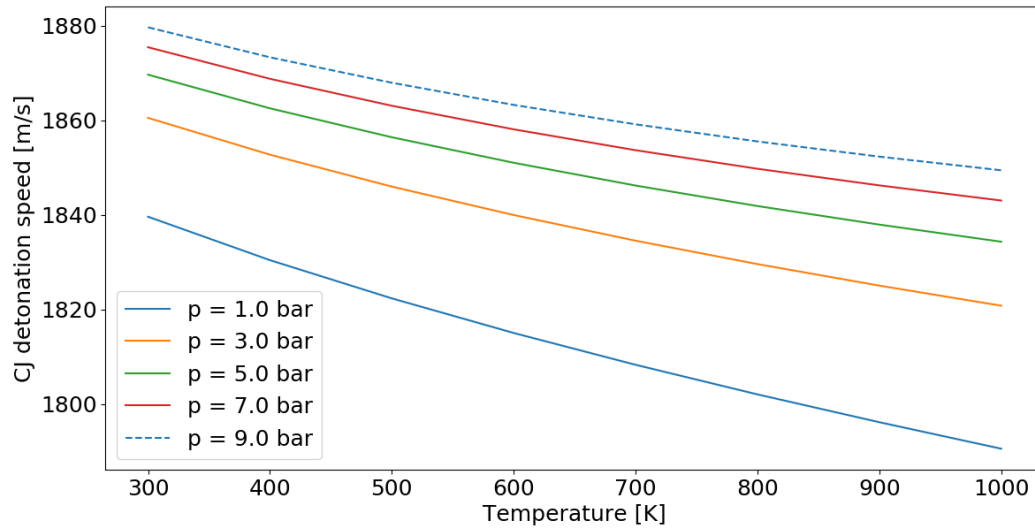


**Figure 4.12.** CJ detonation speed as function of temperature for different initial pressure

$C_3H_7$ :

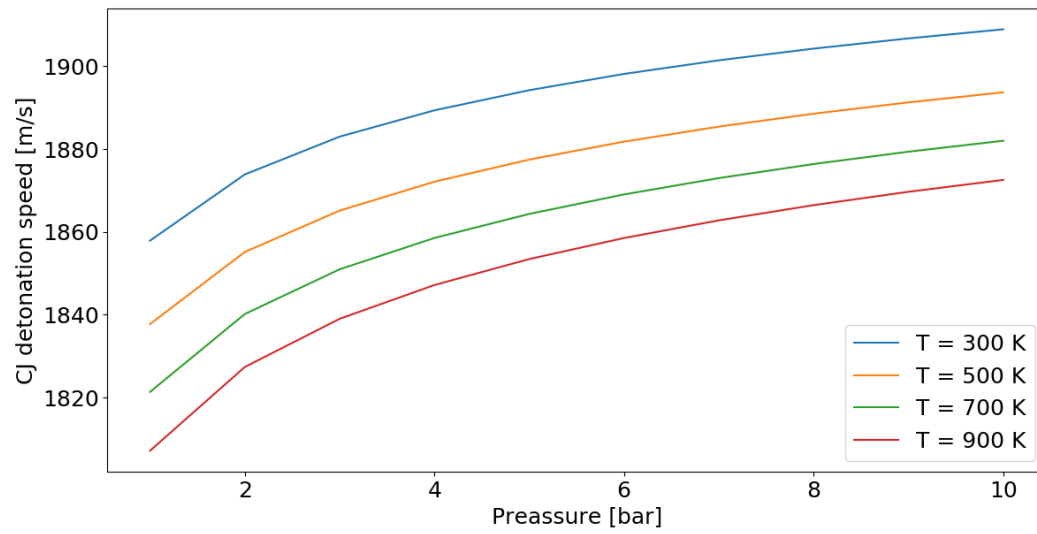


**Figure 4.13.** CJ detonation speed as function of pressure for different initial temperature

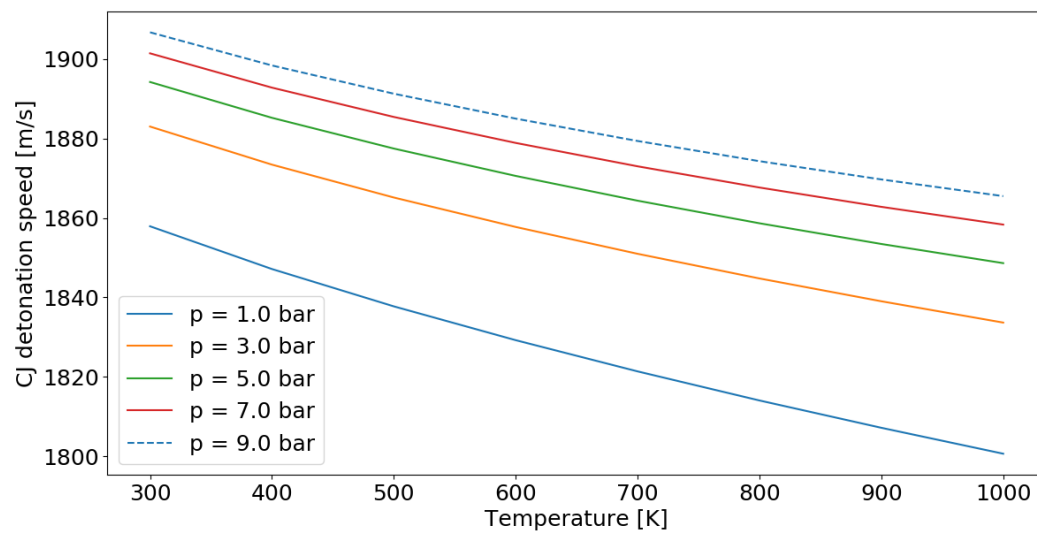


**Figure 4.14.** CJ detonation speed as function of temperature for different initial pressure

$C_2H_2O$ :

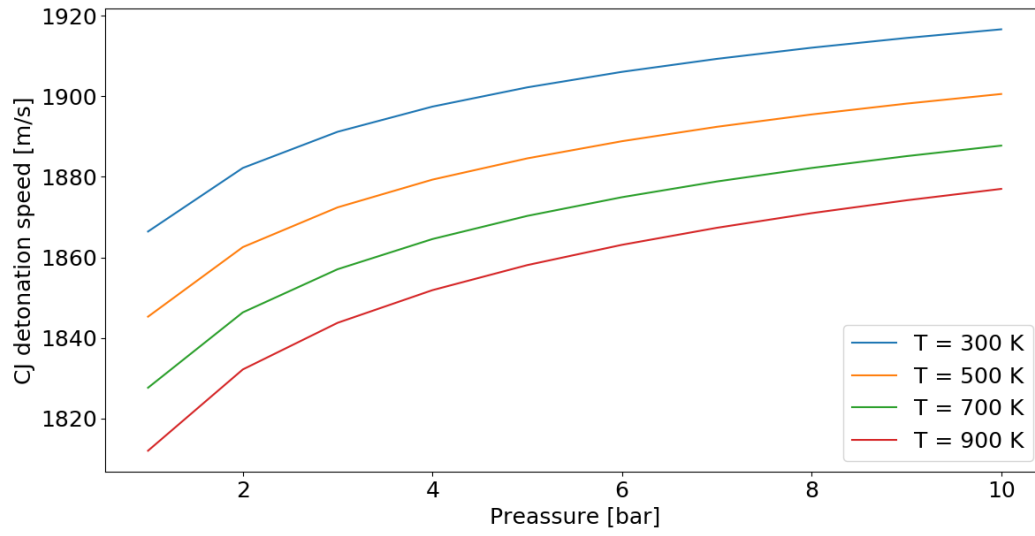


**Figure 4.15.** CJ detonation speed as function of pressure for different initial temperature

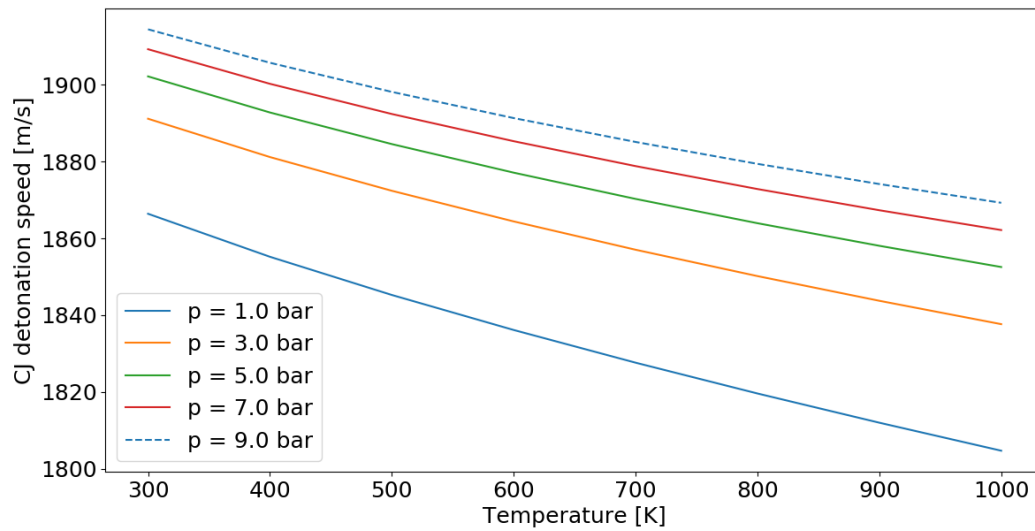


**Figure 4.16.** CJ detonation speed as function of temperature for different initial pressure

$C_2H_2$ :



**Figure 4.17.** CJ detonation speed as function of pressure for different initial temperature



**Figure 4.18.** CJ detonation speed as function of temperature for different initial pressure

## 5. Conclusion

For additional insight, results for analyzed mixtures for the same initial parameters  $P_1 = 1\text{bar}$ ,  $T_1 = 298\text{K}$  are correlated in the chart below.

Mixture	Calculated CJ detonation velocity [ $\text{m/s}$ ]
$H_2 + \text{air}$	1969
$CH_4 + \text{air}$	1803
$C_2H_5 + \text{air}$	1859.8
$C_3H_8 + \text{air}$	1799.8
$C_2H_4 + \text{air}$	1823.8
$C_2H_6 + \text{air}$	1802.6
$C_3H_7 + \text{air}$	1839.8
$C_2H_2O + \text{air}$	1858.1
$C_2H_2 + \text{air}$	1866.7

**Figure 5.1.** Comparison of CJ detonation velocity for nine different mixtures for given initial parameters: pressure 1bar, temperature 298K, equivalence ratio 1

In all cases CJ detonation velocity increases for increasing initial pressure of mixture and on the other hand decreases as the initial temperature rises. The impact of temperature on velocity value is greater for lower initial pressure for each and every mixture. Calculated velocity is the highest for hydrogen premixed with air in stoichiometric amount among all considered processes. The difference between the second highest value, which is  $1866.7 \frac{\text{m}}{\text{s}}$  for  $C_2H_2 + \text{air}$ , totals  $102.3 \frac{\text{m}}{\text{s}}$  and as one can see it appears to be a significant margin.

In order to show how choice of oxidizer impacts obtained velocity value, let's compare stoichiometric mixture of hydrogen and air with stoichiometric mixture of hydrogen and oxygen. CJ detonation velocity for the former is equal to  $1969 \frac{\text{m}}{\text{s}}$  and for the latter to  $2836.3 \frac{\text{m}}{\text{s}}$ . The gap between these two values is almost over one thousand meters per second.

## 6. Sources

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