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Institute of Heat Engineering

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Project

“Influence of gas composition and initial
parameters on C-J detonation’s speed.”

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Chapter 1

Introduction.

1.1. Detonation.

Detonation is a type of combustion involving a supersonic exothermic front accelerating through a medium that eventually drives a shock front propagating directly in front of it. Detonation was discovered in 1881 by two pairs of French scientists Marcellin Berthelot and P. Vieille and Ernest-Francois Mallard and Henry Louis Le Chatelier. Detonations occur in both conventional solid and liquid explosives, as well as in reactive gases. The velocity of detonation in solid and liquid explosives is much higher than that in gaseous ones, which allows the wave system to be observed with greater detail. Gaseous detonations are often associated with a mixture of fuel and oxidant in a composition somewhat below conventional flammability ratios.

The simplest theory to predict the behaviour of detonations in gases is known as Chapman-Jouguet (CJ) theory, developed around the turn of the 20th century. This theory, described by a relatively simple set of algebraic equations, models the detonation as a propagating shock wave accompanied by exothermic heat release. Such a theory confines the chemistry and diffusive transport processes to an infinitesimally thin zone. A more complex theory now known as ZND theory, admits finite-rate chemical reactions and thus describes a detonation as an infinitesimally thin shock wave followed by a zone of exothermic chemical reaction.

1.2. Chapman–Jouguet condition.

The Chapman–Jouguet condition holds approximately in detonation waves in high explosives. It states that the detonation propagates at a velocity at which the reacting gases just reach sonic velocity (in the frame of the leading shock wave) as the reaction ceases. David Chapman and Emile Jouguet originally stated the condition for an infinitesimally thin detonation. A physical interpretation of the condition is usually based on the later modelling by Yakov Borisovich Zel’dovich, John von Neumann, and Werner Doring (the so-called ZND detonation model).

The ZND detonation model is a one-dimensional model for the process of detonation of an explosive. This model admits finite-rate chemical reactions and thus the process of detonation consists of the following stages. First, an infinitesimally thin shock wave compresses the explosive to a high pressure called the von Neumann spike. At the von

Neumann spike point the explosive still remains unreacted. The spike marks the onset of the zone of exothermic chemical reaction, which finishes at the Chapman-Jouguet state. After that, the detonation products expand backward. In the reference frame in which the shock is stationary, the flow following the shock is subsonic. Because of this, energy release behind the shock is able to be transported acoustically to the shock for its support. For a self-propagating detonation, the shock relaxes to a speed given by the Chapman–Jouguet (C-J) condition, which induces the material at the end of the reaction zone to have a locally sonic speed in the reference frame in which the shock is stationary. In effect, all of the chemical energy is harnessed to propagate the shock wave forward. This speed given by the C-J condition is main focus to calculate in this project.

1.3. SDToolbox.

To calculate C-J detonation speed this project will use a SDToolbox library. The Shock and Detonation Toolbox is an open-source software library that enables the solution of standard problems for gas-phase explosions using realistic thermochemistry and detailed chemical kinetics. The SD Toolbox uses the Cantera software package and is implemented as routines that can be called from either MATLAB or Python. A set of demonstration programs and a library of contemporary reaction mechanisms and thermodynamic data are provided. The SD Toolbox includes numerical routines for the computation of:

- CJ detonation speed and post-detonation state
- Postshock gas state for frozen composition
- Postshock gas state for equilibrium composition
- Frozen and equilibrium Hugoniot curves
- Oblique shock waves, shock-expansion solutions
- Shock tube and shock tunnel performance
- Constant-volume explosion structure
- ZND detonation structure
- Effective activation energies and chemical time scales from detailed reaction mechanisms
- Creating and modifying thermodynamic databases.

Chapter 2

Review of the literature.

Shock and Detonation have been studied over the last decades. Many universities and companies were performing research and experiments to better understand the nature of this phenomenon. Calculating the speed of detonation, state of gases after the shock passed and simulating cellular structure of detonation are a main focus of research. At Warsaw University of Technology there is a laboratory (WUT - Combustion Laboratory - Lab 4 - Detonation Burning) where students can perform a controlled detonation, analyze it and compare results with other measurements. For those who don't have an access to this kind of laboratory there is a numerical solution for calculating desired properties. Over the previous 60 years, many numerical solution methods for shock and detonation solutions have been developed and made available as application software. Some of these packages are still in use today, however there are issues with using the older software including limited availability due to national security or proprietary concerns and lack of support for legacy software. In response to this situation a library of software tools, the Shock and Detonation Toolbox have been created and made openly available for students and academic usage. The Toolbox and attached programs are based on the Cantera environment to calculate gas properties, thermodynamics and chemical reactions.

Chapter 3

Model description.

The program calculates the Chapman–Jouguet detonation speed using both Cantera and SDToolbox. The input parameters are initial temperature (and its range to calculate), initial pressure (and its range to calculate) and also the composition of the input gas. This program allows user to calculate how the detonation speed changes with variable fuel, Fuel–air equivalence ratio, addition of nitrogen to the gas composition, initial temperature and initial pressure.

Core of the program is based on demos that have been provided along with SDToolbox package. Used demos are: demo CJ.m and demo CJstate.m . They have been adapted to this project needs by changing the Cantera mechanism to 'gri30.xml' , which allows us to use fuels such as propane, ethane and methane. It also been modified to allow calculations for multiple changing variables. Running the program gives us an output of the detonation speed along with its corresponding case. This data can be used to make plots and see these dependencies.

Chapter 4

Results

4.1. C-J Speed for different fuels.

The fuels used are hydrogen (H_2), methane (CH_4), ethane (C_2H_6) and propane (C_3H_8). They have been detonated in both air ($O_2:1$ $N_2:3.76$ $AR:0.01$) and pure oxygen.

Temperature = 295 K

Pressure = 1000 hPa

Fuel-air equivalence ratio = 1

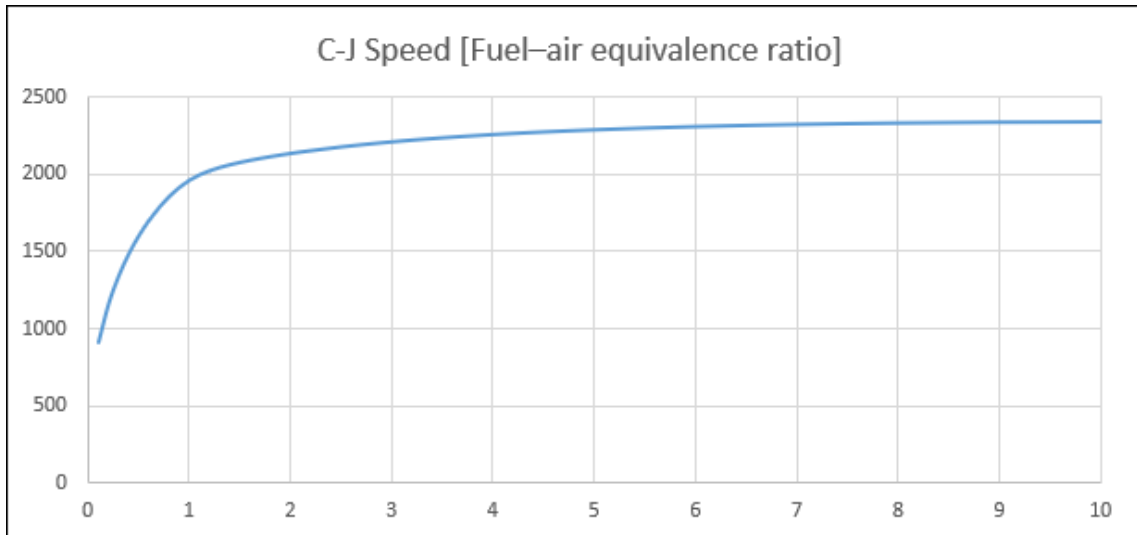
C-J Speed [m/s]		
Fuel	In Air	In Oxygen
H_2	1968,0	2837,2
CH_4	1802,2	2390,7
C_2H_6	1801,8	2369,9
C_3H_8	1799,0	2357,6

In the table above we can see the differences in speed and compare them to actual speed. C-J speed for hydrogen in air should be around 1980 m/s and for HC fuels around 1800 m/s. We can see that hydrogen has a slightly lower speed than expected and HC fuels have speed very similar to each other - it's slightly lower for heavier molecule. We can also see a significant increase in speed if we perform a detonation in pure oxygen. Hydrogen can reach a speed of 2837 m/s.

4.2. C-J Speed for different Fuel–air equivalence ratio.

Fuel–air equivalence ratio is one of the most important variables to consider. In this case we use hydrogen detonating in air. The variable is hydrogen's mole number which varies equivalence ratio from 0,1 to 10.

Temperature = 295 K
Pressure = 1000 hPa
Gas: Hydrogen (H₂) in air



Plot above shows that with increasing equivalence ratio the C-J speed also increases, which is true for hydrogen in this range (equivalence ratio from 0,1 to 10).

4.3. C-J Speed for different nitrogen addition.

Nitrogen does not take part in combustion process. This section shows how adding a non reactive gas changes the speed of C-J detonation.

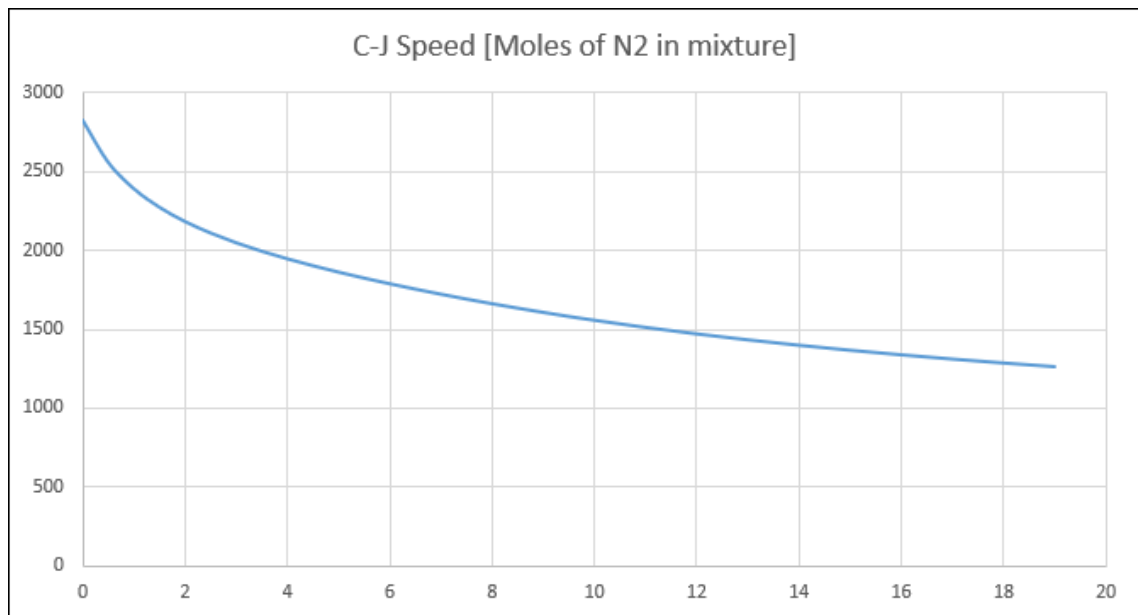
Temperature = 295 K

Pressure = 1000 hPa

Fuel: Hydrogen (H₂)

Equivalence ratio = 1

Gas composition (moles): H₂:2 O₂:1 N₂:variable (from 0 to 19)



Plot above shows that adding a nitrogen to mixture limits the theoretical C-J speed. The speed drops rapidly at the beginning from about 2800 m/s. With huge amount of nitrogen we can see that plot levels out at about 1250 m/s. That's over 2 times lower than without nitrogen at all. We can see a huge influence of nitrogen in detonation speed.

4.4. C-J Speed with variable temperature.

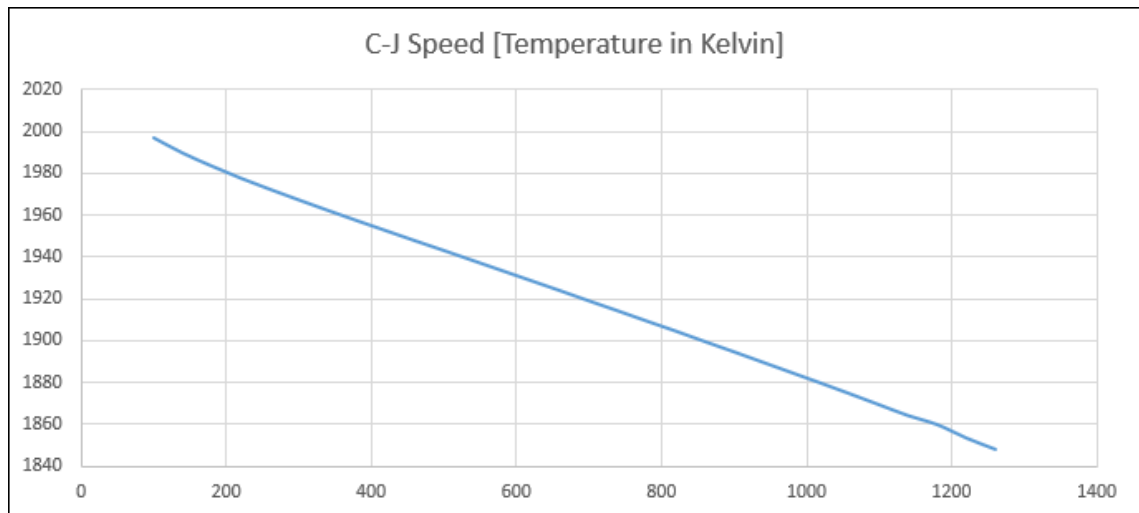
This section shows how initial temperature changes the speed of detonation.

Temperature = variable (from 100K to 1260 K)

Pressure = 1000 hPa

Gas: Hydrogen (H₂) in air

Equivalence ratio = 1

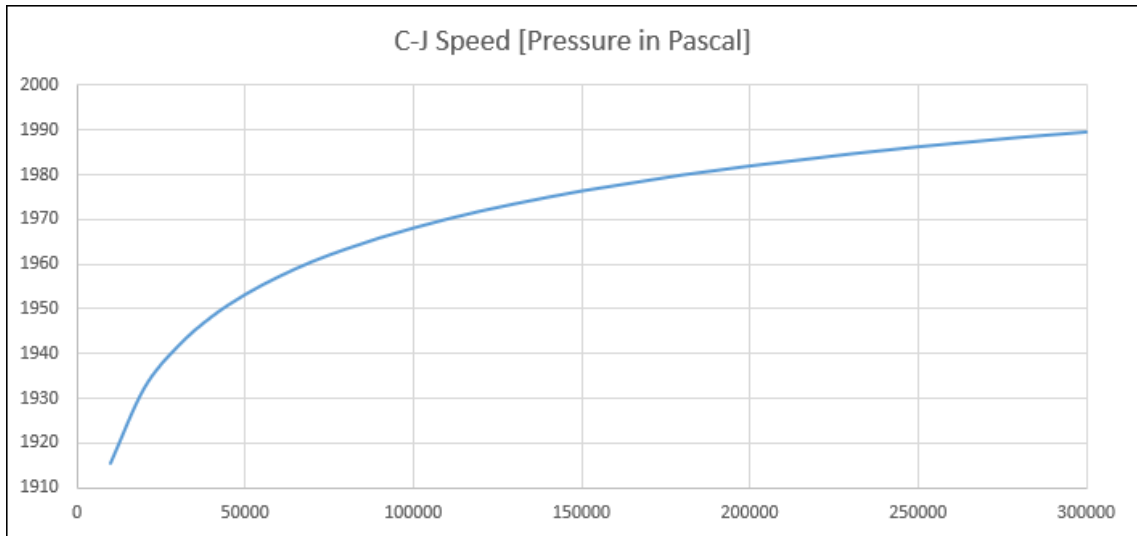


In the plot above we can see almost linear dependence. The higher temperature lowers the detonation speed which is in line with experiments. C-J Speed varies from about 2000 m/s to 1850 m/s, which shows that Temperature does not change the speed that much as adding nitrogen.

4.5. C-J Speed with variable pressure.

This section shows how initial pressure changes the speed of detonation.

Temperature = 295 K
Pressure = variable (from 100 hPa to 3000 hPa)
Gas: Hydrogen (H₂) in air
Equivalence ratio = 1



In the plot above we can see an increase with C-J speed along with increase of pressure. The speed varies from about 1915 m/s to 1990 m/s. Just like temperature, pressure is not that impactful to change the detonation speed, but unlike temperature it increases the speed instead of lowering it.

Chapter 5

Summary and results review.

This model can calculate estimated values of the Chapman-Jouguet detonation speed and predict its changes depending on the variable inputs such as composition and state of initial gas. It accurately shows that the detonation speed increased with increasing Fuel-air equivalence ratio and initial pressure and that detonation speed decreases with increasing temperature and increasing percentage of nitrogen in gas.

Results shows that this model gives predictable results and can be used to roughly calculate the C-J speed. The calculations are close to experiments result's but still this should be used only to estimate the detonation speed because this model assumes ideal conditions that can't consume the shock and detonation energy.

List of Sources.

- <https://cantera.org/tutorials/python-tutorial.html>
- <https://cantera.org/documentation/docs-2.4/sphinx/html/cython/thermo.html>
- <https://matplotlib.org/>
- <https://docs.scipy.org/doc/numpy-1.15.0/user/basics.creation.html>
- <http://cs231n.github.io/python-numpy-tutorial/>
- <https://treyhunner.com/2016/04/how-to-loop-with-indexes-in-python/>
- <https://en.wikipedia.org/wiki/Detonation>
- https://en.wikipedia.org/wiki/Chapman-Jouguet_condition
- <http://shepherd.caltech.edu/EDL/PublicResources/sdt/>
- SDToolbox Quick REference SDT
- WUT - Combustion Laboratory - Lab 4 - Detonation Burning