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POWER AND AERONAUTICAL ENGINEERING

Institute of Heat Engineering

in the field of study Aerospace Engineering
and specialisation Aircraft Propulsion

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 (from Latin detonare, meaning 'to thunder down/forth').It 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 Joguert 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 beed 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) were student can perform a controlled detonation, analize it and compare results with other measurements. For those who don't have an access to this kind of laboratory there is an numerical solution for calculating desired propeties. 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 avaliable for students and academic usage.The Toolbox and attached programs are based on the Cantera enviroment to calculate gas propeties, thermodynamics and chemical reactions.

Chapter 3

Model description.

The program calculates the Chapman–Jouguet detonation speed using both Cantera nad SDToolbox. The input parameters are intial temperature (and it's range to calculate), intial pressure (and it's 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, intial temperature and intial pressure.

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

Chapter 4

Results

4.1. C-J Speed for diffrent fuels

The fuels used are hydrogen (H2) , methane (CH4), ethane (C2H6) and propane (C3H8). The have been detonated in both air (O2:1 N2:3.76 AR:0.01) and pure oxygen.

Temperature = 295 K
Pressure = 1000 hPa
Fuel–air equivalence ratio = 1

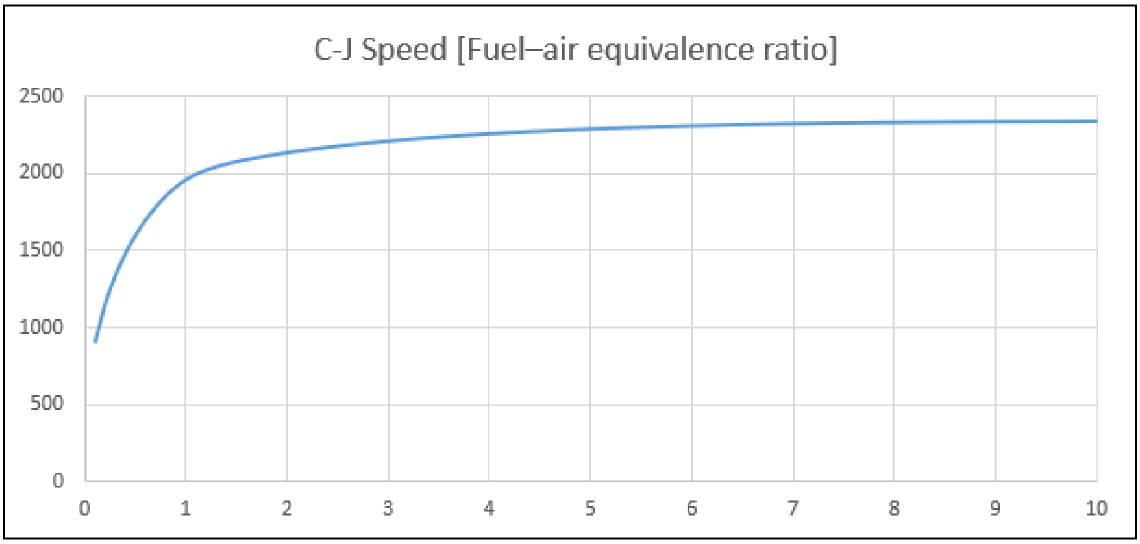
C-J Speed [m/s]		
Fuel	In Air	In Oxygen
H_2	1968,0	2837,2
CH_4	1802,2	2390,7
C_2H_6	1801,8	2369,9
C_3H_8	1799,0	2357,6

In the table above we can see the diffrences 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 diffrent 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

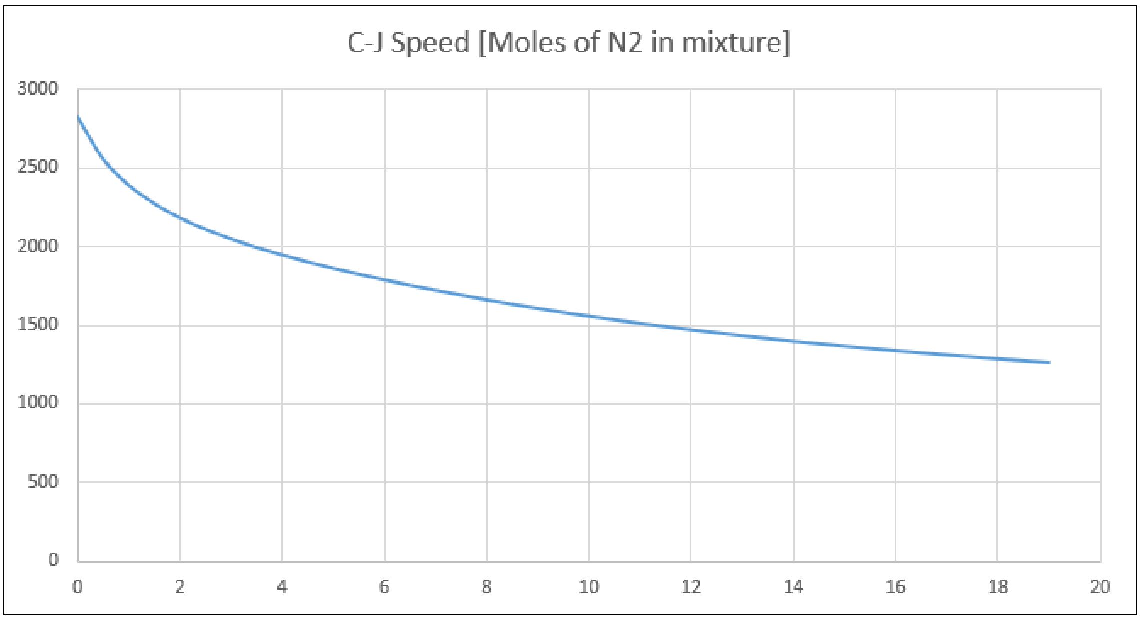


Plot above shows that with increasing equivalence ratio the C-J speed also increases, witch is true for hydrogen in this range (equivalence ratio from 0,1 to 10).

4.3. C-J Speed for diffrent nitrogen addition

Nitrogen does not take part in combustion precess. 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)

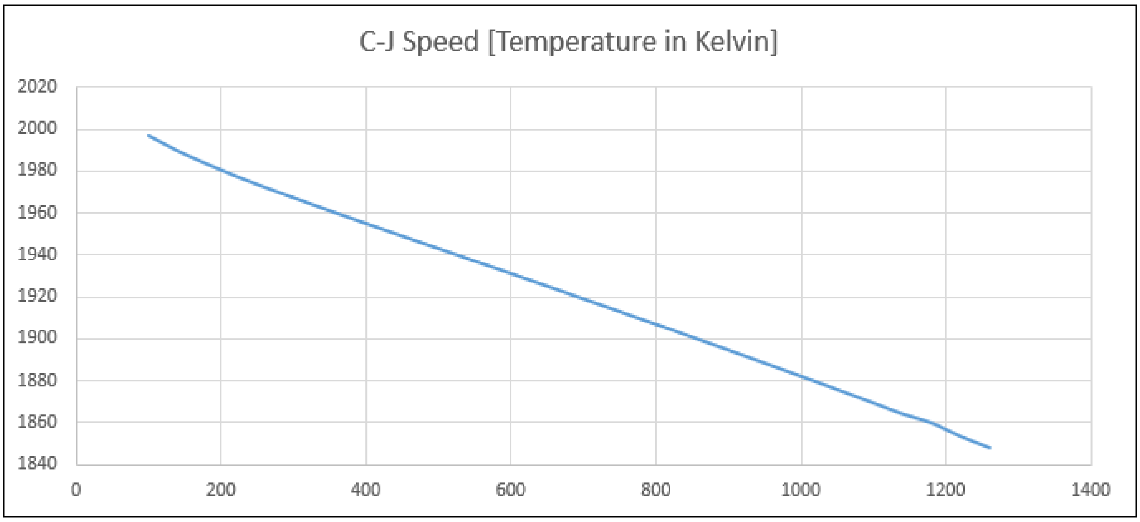


Plot above shows that adding a nitrogen to mixture limits the theoretical C-J speed. The speed drops rapidly at the beginning from about 2800 m/s. With huge amount of nitrogen we can see that plot levels out at about 1250 m/s . That's over 2 times lower than without nitrogen at all. We can see a huge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

4.4. C-J Speed with variable temperature

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

Temperature = variable (from 100K to 1260 K)
Pressure = 1000 hPa
Gas: Hydrogen (H2) in air
Equivalence ratio = 1

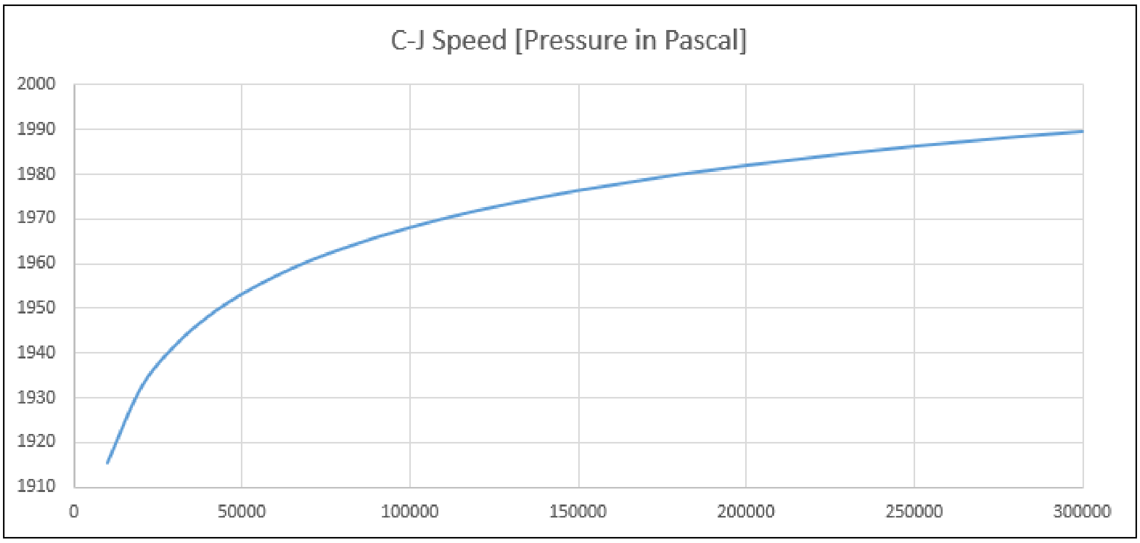


In the plot above we can see almost linear dependence. The higher temperature lowers the detonation speed with is in line with experiments. C-J Speed varies from about 2000 m/s to 1850 m/s, witch shows that Temperature does not change the speed that much as adding nitrogen.

4.5. C-J Speed with variable pressure

This section shows how intial 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 it's changes depending on the variable inputs sush as composition and state of intial gas. It accurately shows that the detonation speed increased with increasing Fuel-air equivalence ratio and intial pressure and that detonation speed decreases with increasing temperature and increasing precentage of nitrogen in gas. Results shows that this model gives predictable results and can be used to roughly calculate the C-J speed.

List of Sources.

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- https://matplotlib.org/
- https://docs.scipy.org/doc/numpy-1.15.0/user/basics.creation.html
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- https://en.wikipedia.org/wiki/Detonation
- https://en.wikipedia.org/wiki/Chapman–Jouguet condition
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- WUT - Combustion Laboratory - Lab 4 - Detonation Burning