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Course: Aerospace Engineering (PL)

Numerical calculation of parameters of an air – propane mixture after detonation, using SDToolbox

Contents

1. Introduction

Detonation is a type of combustion involving supersonic exothermic front accelerating through a medium that eventually drives a shock front propagating directly in front of it. It is a process composed of two physical phenomena, interacting with each other but treated separately: compression in shock wave and combustion. The combustion products travel in the same direction as the shock wave. Both pressure and density increase during this process.

The way a normal combustion turns into a detonation is shown on Fig. 1. The combustion occurs at the closed end of the chamber, a laminar flame propagates through the chamber. Combustion products are situated between the front of the flame and closed end of the chamber. Those products expand. By doing so they push the mixture ang generate pressure waves which in turn overlap, because each wave travels in an ambient with a higher temperature. At a certain point those pressure waves become one shock wave, the temperature of which is higher than the temperature of ignition of the mixture. After the time of ignition has passed, ignition and then heat explosion occur.

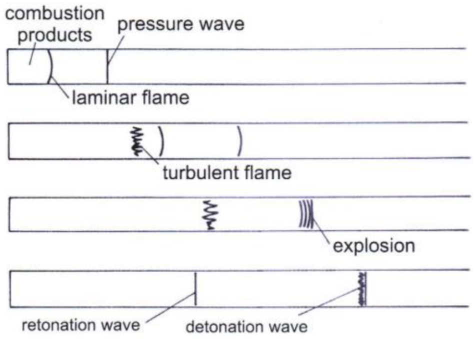

Fig. 1 Cartoon representing the process of detonation [1]

The properties explored in this report are:

- Post shock wave temperature vs initial fuel to mixture concentration, pressure and temperature
- Post shock wave pressure vs initial fuel to mixture concentration, pressure and temperature
- Chapman – Jouguet speed vs initial fuel to mixture concentration, pressure and temperature

The Chapman – Jouguet speed is the minimum velocity at which a stable detonation wave travels.

Understanding how those parameters change helps implementing detonation in several applications such as: explosives, projectiles, deposition of coatings, cleaning of equipment, explosive welding. It is also important in order to prevent detonations and estimate the risk they pose in mines.

Mathematical model and code analysis

Numerical solution methods were used to calculate the properties of shock and detonation properties. The region far downstream form the shock wave is considered in thermodynamic equilibrium. The mathematical model is deeply explored in [2]. Both Cantera and SDToolbox software tools were implemented. The GRI – Mech 3.0. chemical reaction mechanism was also used. The way it works is rigorously explained on the GRI – Mech website [3] and other papers published by The University of California, Berkeley, Stanford University, The University of Texas at Austin and SRI international. For the sake of simplicity of this report, the elaboration on how GRI – Mech works and the mathematical model of numerical calculations of detonation properties is omitted on purpose. Any reader who is interested in the topic is invited to visit the mentioned positions. The code written to perform the calculations was based on the one published as demo on the SDToolbox website [4], called *demo_CJstate.py*.

The code consists of # major parts

I. Declaration of values of initial parameters, and arrays of initial parameters.
II. 3 Cores of the code, which are responsible for the calculations. The user may decide which calculations to perform i.e. which initial parameter is to be set as variable, while the rest are held constant.
III. Plotting the results

Since every core is almost identic, only one will be analysed in this report:

`for C1 in C_array:`	C1 – initial concertation value; C_array – evenly spaced concertation values, which are in the propane flammability range
`a = 4.76 * C1 / (1 - C1)`	a – number of propane moles
`q = 'O2:1.,N2:3.76,C3H8:' + str(a)`	Declaration of the mixture
`[cj_speed, R2] = CJspeed(P1, T1, q, mech, 0)`	Computation of the CJ speed
`gas = PostShock_eq(cj_speed, P1, T1, q, mech)`	Computation of the post shock wave state

`P2.append(gas.P * 0.00001)`
`T2.append(gas.T)`
`CJspeedo.append(cj_speed)`
	Adding the calculated parameters to arrays for future display

2. Results and discussion

2.1. Variable initial fuel to mixture concertation, constant initial temperature (300 K) and pressure (1 bar)

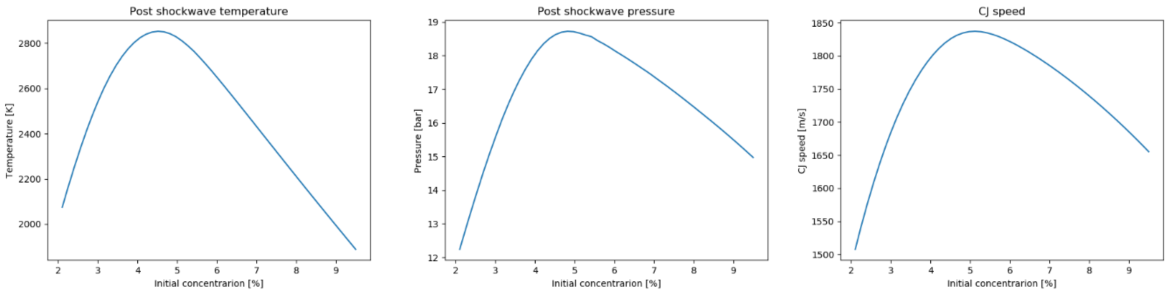

Fig. 2 - 4 Influence of initial fuel to mixture concentration on post detonation shockwave state

The concentration of fuel plays a key role in the process of detonation combustion. One can observe that all three of the calculated parameters have a peak at ≈ 4 % propane concertation, which is the ideal (stoichiometric) ratio in the combustion of propane in air.

2.2. Variable initial pressure, constant initial temperature (300 K) and fuel to mixture concentration (4%)

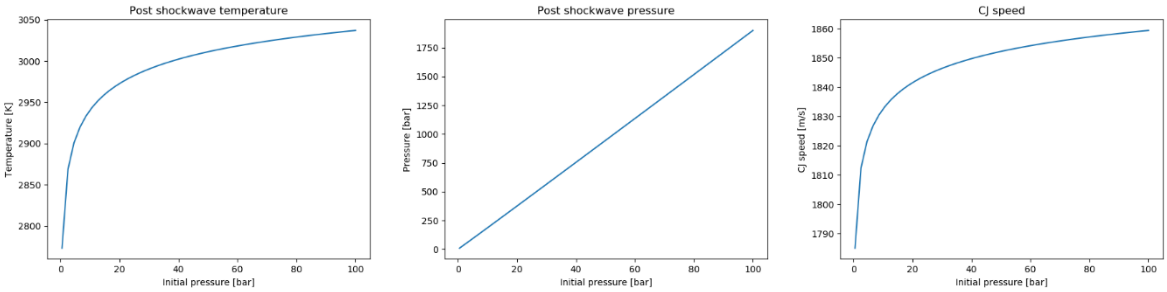

Fig. 5 – 7 Influence of initial pressure on post detonation shockwave state

All parameters increase with initial pressure. Both temperature and CJ speed have a quite big gradient for pressures in range from 0.5 bar to 20 bar, then it seems to die out. Post shockwave pressure, however has a linear relation to initial pressure.

2.3. Variable initial temperature, constant initial pressure (1 bar) and fuel to mixture concentration (4%)

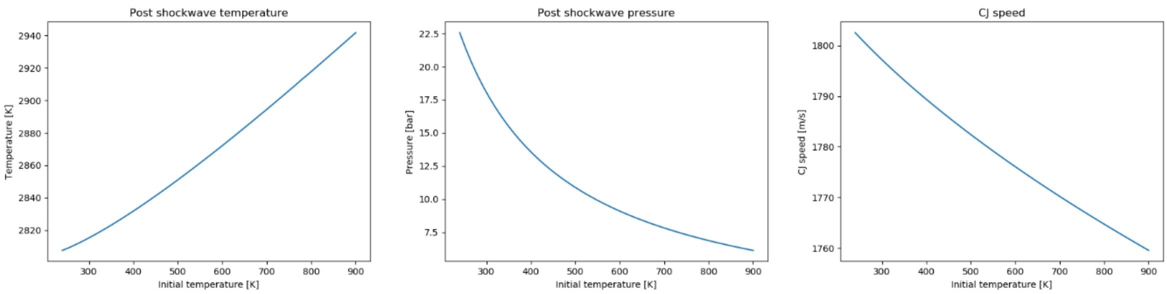

Fig. 8 – 10 Influence of initial temperature on post detonation shockwave state

In this case only post shock wave temperature increases with initial temperature. Post shockwave pressure has a steeper slope compared with CJ speed.

3. Conclusions

- Initial temperature, pressure and concentration have an impact on the process and the outcome of a detonation combustion.
- With the increase of the fuel concentration, the post shock wave temperature, pressure and CJ speed increase until it reaches the stoichiometric ratio. After that all three parameters drop.
- The increase of initial pressure results in the increase of all three examined parameters.
- The higher the initial temperature is the lower is the post shockwave pressure and CJ speed, in contrast to post shock wave temperature.
- In order to minimize the Chapman – Jouguet speed (speed at which a detonation propagates) one has to increase the initial temperature, reduce initial pressure and have the fuel concentration stand far from the stoichiometric ratio. Since out of the laboratory it is difficult to alter both pressure and temperature, especially in mines, in order to keep a safe environment it is crucial to constantly observe the concentration of potential fuels in the air, and be aware of their flammability range.

4. References

[1] Dr. hab. Marian Gieras lecture on detonation and deflagration
[2] S. Browne, J. Ziegler, and J. E. Shepherd *"Numerical Solution Methods for Shock and Detonation Jump Conditions"*
[3] GRI – Mech project overview: *http://combustion.berkeley.edu/gri-mech/overview.html*
[4] The SDToolbox website http://shepherd.caltech.edu/EDL/public/cantera/html/SD_Toolbox
[5] Basic information on detonation *https://en.wikipedia.org/wiki/Detonation*
[6] Author's github repository: *https://github.com/MathiaFiorelli/MKWS*