Chapman Jouguet Speed and Postshock State

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1 Introduction

There are two modes of combustion propagation in gas mixtures. In slow combustion mode gas burns in flame front, velocity of which is defined by transition processes: heat conductivity and diffusion. During detonative combustion mode compression and heating of combustible mixture, which lead to its ignition, are carried out by shock wave of high intensity. In this case the combustion is localized inside of narrow area behind shock wave, so it has the same as shock wave velocity which can reach up to few kilometers per second. Interest in the detonation combustion has recently increased. This is due to the development of detonation engines, which are superior to all other types of heat engines in terms of thermodynamic efficiency. A lot of reviews of studies of detonation were made. Below, the detonation of a mixture of hydrogen and air will be analided. When burnt with clear oxygen, hydrogen is a "zero-emission" fuel, which means that there will be no waste products after the combustion. However, while burning in atmospheric air, hydrogen combustion may yield small amounts of nitrogen oxides. This kind of fuel is used in many cases, such as passenger cars, fuel cell buses and even spacecraft. The aim of this simulation is measurement the Chapman Jouguet speed for a mixture of air and hydrogen. There will be considered how it changes depending on initial external conditions and also check the state of a gas after detonation.

2 Literature

Literature which was used here is:

-wikipedia.org

-Numerical Solution Methods for Shock and Detonation Jump Conditions.

3 Description of Chapman Jouguet

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 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 Dring - authors of a ZND detonation model.

The aim of this project is mainly to calculate the CJ speed. CJ speed can be defined as follows:

Definition: The Chapman-Jouguet detonation velocity is the minimum wave speed for which there exists a solution to the jump conditions from reactants to equilibrium products traveling at supersonic velocity. The minimum wave speed condition occurs when the Rayleigh line is tangent to the Hugoniot.

3.1 Detailed CJ state analysis for three different gases with three different initial conditions

In this project it was said that the gas should be a mixture of hydrogen and air. The fractions of each component was decided to be constant for every gas in this project and they were:

H2 = 0.7

Air = 1 = (O2 = 1, N2 = 3.76)

To check the differences between different initial conditions there are three gases with the same reactants but with different temperatures and pressures. There will be used h2air high T mechanism.

The first gas (gas1) has tempterature T = 300 K and pressure p = 1 atm. The second gas (gas2) has tempterature T = 300 K and pressure p = 1.5 atm. The third gas (gas3) has tempterature T = 400 K and pressure p = 1 atm.

After calculations we achieved many information about the state of mixture after detonation, CJ speed and also equilibrium and frozen velocities of sound. The simulation is using Cantera, which is a software tool for Python language with addition of SDToolbox that is a shock and detonation package for Cantera. All is shown below:

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For H2:0.7, O2:1, N2:3.76 in the first case: P1 = 100000.00 Pa & T1 = 300.00 K u
sing h2air_highT.cti
CJ Speed is 1423.09 m/s

For H2:0.7, O2:1, N2:3.76 in the second case: P1 = 150000.00 Pa & T1 = 300.00 K
using h2air_highT.cti
CJ Speed is 1423.20 m/s

For H2:0.7, O2:1, N2:3.76 in the third case: P1 = 100000.00 Pa & T1 = 400.00 K u
sing h2air_highT.cti
CJ Speed is 1433.03 m/s
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Figure 1: CJ speed for three different gases.

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The CJ State for the first case is 952642.18 Pa & 1791.43 K

The CJ State for the second case is 1429076.83 Pa & 1791.68 K

The CJ State for the third case is 737547.15 Pa & 1870.99 K
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Figure 2: CJ state for three different gases.

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The sound speeds for the first case are: af1 = 838.76 m/s & ae1 = 834.82 m/s

The sound speeds for the second case are: af2 = 838.81 m/s & ae2 = 834.97 m/s

The sound speeds for the third case are: af3 = 856.45 m/s & ae3 = 851.36 m/s
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Figure 3: Parameters for three different gases. Index f means frozen and e means equilibrium. These two different sound velocities are quite similar.

3.2 CJ speed and postshock parameters depending on initial pressure

The next part of this project was to calculate CJ speed and postshock parameters as a function of initial pressure. There were 10 measurements increasing pressure of 1 atm. The first initial pressure was set to 0,1 MPa, which is close to one atmosphere. The rest of parameters, temperature and mole composition, were constant.

Results can be seen on both arrays and figures:

Pressure [atm]	CJ speed [m/s]
1.0	1609.1
2.0	1610.4
3.0	1611.0
3.9	1611.4
4.9	1611.7
5.9	1612.0
6.9	1612.2
7.9	1612.3
8.9	1612.4
9.9	1612.6

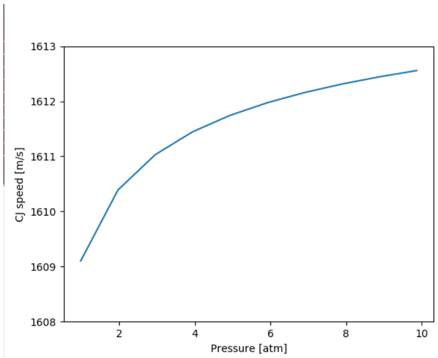

Figure 4: CJ speed is rising alond with pressure.

During calculations program saved also parameters of gas after shockwave for every initial pressure. The most important parameters are pressure and temperature after detonation and so they are gathered together in a combined array:

Pressure [atm]	Post Shock pressure [atm]	Post Shock temperature [K]
1.0	11.5	2201.7
2.0	23.0	2205.0
3.0	34.5	2206.7
3.9	46.0	2207.6
4.9	57.5	2208.4
5.9	69.1	2208.9
6.9	80.6	2209.4
7.9	92.1	2209.8
8.9	103.6	2210.1
9.9	115.1	2210.4

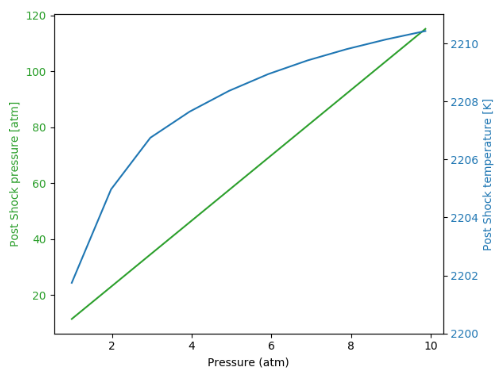

Figure 5: Temperature of gas rises similarily to CJ speed. On the other side pressure rises linearly. For about 7 atm we have gas pressure about 80 atm. This kind of value is measured in a piston after work stroke in an engine.

3.3 CJ speed and postshock parameters depending on initial temperature

These calculations are similar to previous ones, the only difference is that the pressure is constant and equals 1 atm, while the temperature will be changed. First temperature is set to 300 K and 10 times it is rised of 100 K. Pressure and mole compositions remains the same for every measurement. Results may be seen below:

Temperature [K]	CJ speed [m/s]
300.0	1610.5
400.0	1609.4
500.0	1608.3
600.0	1607.3
700.0	1606.2
800.0	1605.1
900.0	1604.1
1000.0	1603.0
1100.0	1601.9
1200.0	1600.8

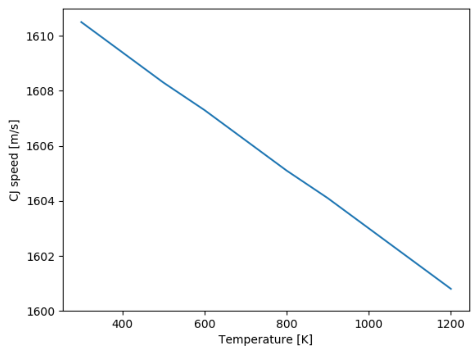

Figure 6: There can be seen that CJ speed decreases linearly in whole range of temperatures.

Temperature [K]	Post Shock pressure [atm]	Post Shock temperature [K]
300.0	11.5	2201.7
400.0	8.8	2269.2
500.0	7.2	2334.3
600.0	6.1	2397.2
700.0	5.3	2457.8
800.0	4.7	2516.0
900.0	4.3	2571.9
1000.0	3.9	2624.9
1100.0	3.6	2674.9
1200.0	3.3	2720.8

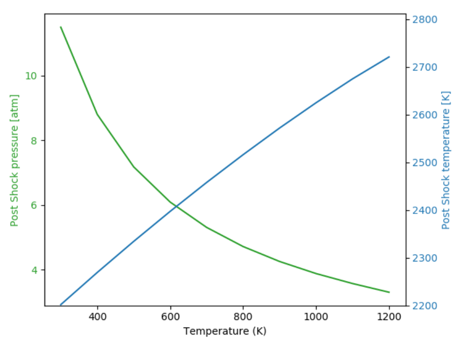

Figure 7: Results are different from previous calculations. Pressure decreases while in the previous case it increased, but CJ state temperature rises. For a temperature that occurs in nowadays turbine engines there is a value of about 2600 K. It is such high that only very few materials can bear.

4 Summary

As we can see CJ speed strictly depends on both initial pressure and initial temperature. Moreover, postshock parameters (pressure and temperature) depends on both initial values as well. From both introduction and description we can surely say that CJ speed and postshock parameters are very important parameters in nowadays combustion.