Influence of equivalence ratio on reaction zone induction time, detonation cell size and C-J speed of hydrogen-air mixtures

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1 Detonation theory

There are numerous detonation models in use in the scientific community which aid in the understanding of the processes governing this phenomenon. Two of them: Chapman-Jouguet's model (C-J) and Zeldovich-Neumann-Doring model (Z-N-D) are the most prevalent. While C-J presents a somewhat simplified yet still useful picture of a detonation, Z-N-D model is far more intricate and utilizes more input parameters.

According to the C-J theory, the detonation wave moves at a constant velocity at which the reactants reach the speed of sound. The shockwave itself is modeled as a discontinuity in the medium. C-J does not take into consideration the chemical kinetics of the reaction, but it allows the calculation of the speed and the pressure of the shockwave. The speed of the wave calculated using C-J theory is referred to as the C-J speed.

Z-N-D model is a more realistic approach which allows us to describe the detonation more precisely. Using C-J speed and pressure as inputs along with information about the chemical kinetics of the reactions, we are now able to calculate both the length of the reaction zone and the induction time of the reaction zone. These two parameters are governed by the chemical kinetics which characterize each and every fuel-oxidizer mixture.

Every detonation has a multidimensional cellular structure which is often determined through experiments. The size of detonation cells is closely determined by several parameters such as activation energy and critical diameter of the experimental tube. The results of such tests can be found in detonation cell size databases.

One of the most significant initial parameters influencing the detonation is the equivalence ratio of the fuel-oxidizer mixture which is the ratio of the actual fuel-to-air ratio (FAR) of the mixture to stoichiometric FAR.

$$FAR = \frac{n_{fuel}}{n_{air}}$$
$$\phi = \frac{FAR}{FAR_{stoichiometry}}$$

φ greater than one means that the mixture is rich and not all of the the fuel undergoes combustion due to lack of oxidizer. Alternatively, φ lower than one indicates a lean mixture which has an excess of oxidizer.

2 Methodology

The aim of the simulation was to determine the influence of equivalence ratio on the induction time and C-J speed of hydrogen-air mixture ignition as well as to find the correlation between said induction time and detonation cell size. The simulation was run in two parts: Task 1 (C-J speed as a function of equivalence ratio) and Task 2 (induction time and cell size correlation) which both utilized Cantera suite for chemical kinetics calculations in Python and SD Toolbox.

Task 1 was completed using a straightforward SDToolbox/Cantera/Python script which uses set temperature (300K) and pressure (100 kPa) as input. These initial conditions were deemed easiest to compare with existing data. The script then runs a loop which sets the composition of the hydrogen-air mixture and calculates C-J speed for given equivalence ratio. The loop starts with a molar fraction of hydrogen equal to equivalence ratio of 0.1, rising by 0.1 each increment up to 2.5.The results are appended to an array and plotted using matplotlib library. Source code of task 1 also includes a loop creating input files for ZND software which ultimately remained unused (a simpler solution was used) but was left as an exercise in Python coding which may be useful in future projects.

Task 2 used a combination of Cantera-and-ZND-enabled MATLAB script. Integration of ZND software and said MATLAB script proved to be exceedingly cumbersome and time-consuming due to extremely limited documentation, thus a semi-manual method was devised. C-J speeds and induction times which were calculated by ZND for given equivalence ratio were manually copied directly to a spreadsheet. This data was then used to calculate and find the maximal induction time gradient over equivalence ratio. Using a detonation cell size database, a set of data for the given conditions was found (Cell size for the equivalence ratio at which maximal induction time gradient occurred was used to calculate a correlation coefficient.Additionally, C-J speeds calculated here were compared with the results of Task 1.

3 Results

3.1 Task 1 - C-J speed vs equivalence ratio

Task 1 results are presented in Fig. 1. The Chapman-Jouguet speed of detonation wave rises quasi-logarithmically with equivalence ratio. It appears to have a horizontal asymptote of around 2200 m/s. The calculated values fit between 900 m/s for equivalence ratio of 0.1 and 2200 m/s for 2.5 in a direct exponential correlation between initial pressure and autoiginiton temperature (Figure 1).

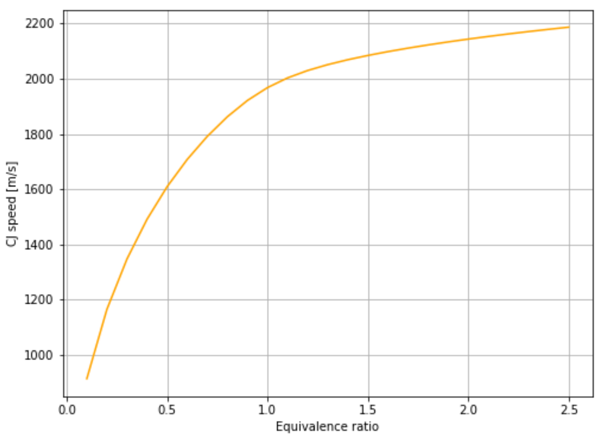


Figure 1: Results of Task 1. C-J speed as a function of equivalence ratio calculated using SDToolbox in Python

3.2 Task 2 - induction time vs equivalence ratio; detonation cell size

Results of reaction zone induction time calculation are presented in Fig. 2. The highest gradient of this time over equivalence ratio was determined to be achieved at equivalence ratio 0.6-0.7.

$$\frac{dt_{ind}}{d\phi} = 7,33 * 10^{-6} \frac{s}{1}$$

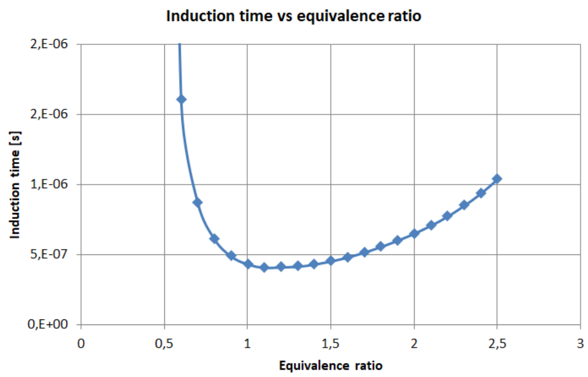


Figure 2: Results of Task 2. Reaction zone induction time calculated using SDToolbox in MATLAB

According to 1994 research of G. Cicarelli, detonation cell size at these initial conditions and equivalence ratio equals 41,48 mm. This value was subsequently used to calculate the correlation coefficient between detonation cell size and reaction zone induction time.

$$\lambda = a * t_{ind}$$

$$a = \frac{\lambda}{t_{ind}} = \frac{41,48}{1,6 * 10^{-6}} = 2,59 * 10^{7} \frac{mm}{s}$$

Applying this coefficient to calculated induction times resulted in cell sizes for all studied equivalence ratios as presented inf Fig. 3.

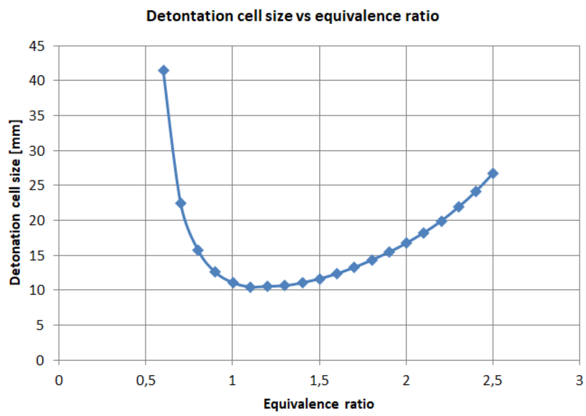
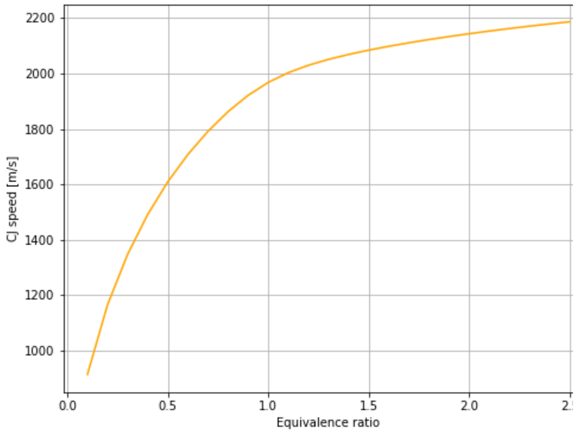


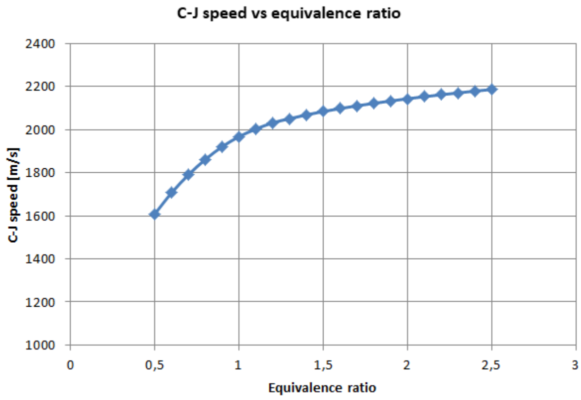
Figure 3: Results of Task 2. Detonation cell size calculated using correlation coefficient determined previously

Minimal cell size of 10mm was achieved at equivalence ratio of 1.1.

In order to validate these results, C-J speeds calculated using MATLAB script were also compared with previous results of Task 1.



(a) CJ using SDT in Python



(b) CJ speed using SDT in MATLAB

Figure 4: Comparison of C-J speeds calculated using different methods

Results of both methods match each other, therefore the calculations are correct.

4 Conclusions

Chapman-Jouget speed rises quickly with equivalence ratio for lean mixtures and slowly for rich mixtures. The speed appears to reach an asymptote of 2200-2300 m/s.

The lowest reaction zone induction times are reached for equivalence ratios close to stoichiometric. Enriching a lean mixture lowers the induction time. Enriching an already rich mixture raises it. The highest induction time gradient can be observed for lean mixtures of equivalence ratio around 0.6-0.7. In comparison, rich mixtures display lower gradients. Detonation cell size directly corresponds to induction times, therefore they are minimal when the induction time is minimal.

5 References

1. Anne Felden, *CANTERA Tutorials*, Tutorial 4, CERFACS, November 2015

2. John von Neumann, *Theory of detonation waves. Progress Report to the National Defense Research Committee Div. B*, April 1942, New York

3. Rafał Porowski, *Wprowadzenie do procesów spalania*