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Project of SD Toolbox
Computer Methods in Combustion

THE DETONATION ANALYSIS

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1 Abstract

Computation of detonation wave parameters was carried out using SDToolBox with Cantera software. Detonation cell size were predicted, and maximum pressure was calculated for hydrogen – air mixture detonation. Results were compared with experimental data.

2 Introduction

Following ignition of a steady, homogenous air – hydrogen mixture, kinetic flame front propagates and after some distance travelled, chances are for it to undergo deflagration – detonation transition. Phenomenon usually requires large volumes and spaces to take place however it can be reproduced inside a lab using special pipe with flame front turbulence inducing steel mesh. Process of flame propagation inside the pipe filled with homogenous air – fuel mixture can be divided into few steps. At the beginning of combustion there is an undisrupted laminar flame propagating after weak pressure wave. As flame front gets turbulised, the combustion rate increases, so as thermal energy production rate and pressure gain before the reaction region. This air compression and radiation heating causes temperature rise in unreacted mixture rendering it easier to burn as less energy shall be introduced to it inside the reaction zone. As a result – flame propagation velocity increases along with pressure wave intensity in a closed, self-boosting loop, until it exceeds the speed of sound in non-reacted mixture while undergoing deflagration – detonation transition. Usually cellular detonation occurs with cell size corresponding with how fast the chemical reaction takes place. The detonation cells can be visualised inside the pipe by using a flat plate covered with carbon soot laid along the wall. The smaller the cells are, the more vigorous reaction was. Using SDToolBox with Cantera Software, there was a prediction made on how maximum pressure behind the detonation wave and the cell size depends on the air – fuel mixture composition, expressed as equivalence ratio, in a steady state conditions.

3 Models

3.1 Experimental models

The aim of experiment was to cause delfagration – detonation transition in longitudinal steel pipe (sizing: 0,11 x 0,8 x 2), and check reactivity of homogenous air – fuel mixture by measuring size of detonation cells. The clearest cells (best for measuring) appear in end of tube. It is caused by tendency to increase reaction's intensivity as the wave approaches the end of the tube, where measuring equipment is located. In fact, those dimensions are too small to allow the flame to achieve appriopriate valocity for desirable transition. To reduce time needed for the flame to accelrate, just behind ignition was located the net of steel aimed to turbulise the flow, what greatly suppotrs development of „self-boosting detonation loop" which was previously mentioned. For comparison: in normal conditions to cause detonation combustion the pipe shuld be at least three times longer. For measuring flow velocity and pressure in apparatus were placed two pairs of sensors: Piezoelectrical for pressure, and ionisation for checking location of the flame in time. Signals form sensors were multiplied by properly calibrated signal amplifier, and subsequently written in previously prepared file. Due to high frequency of data sampling – 2MHz, and limited data capacity of mentioned file, very important thing is to synchronise the moment of ignition with the moment when the measurment is started. So as to, in addition, extra sensors were added in the area behind the net. They were proggramed to send a signal initialising the sampling. Another significant part of experiment is to place a sooted plate at the end of the pipe which can be used to examine and measure created detonation cells.

3.2 Computation model

Simulation commited during creation of this project was based on rather simple programme providing results on estimated detonation cell size and thermodynamical parameteres in the nearest vicinity of reaction zone. Situation created to run experiment had to be simplified to adapt it to Cantera's functions. The main difference is fact, that numerical simulation was held in zero-dimensional environment, not inside pipe with determined dimensions. The chosen solution was performed with Mevel2017 chemical kinetic mechanism, a resource delivered by California University of Technology, alongside SD Toolbox library for Cantera. It's array of chemical reactions dedicated to depict thermal state of hydrogen-air mixture and dynamics of its combustion. Mentioned numerical engine was not sufficient however to simulate complicated structure of detonation wave and zones it's composed of. To provide more advanced algorithm, library containing ZND mechanism was imported. ZND theory enabled cell size (according to Gavrikov's correlation) to be estimated as well as reaction zone's width. As for the formal side of the problem, a number of Cantera objects were used to hold data while computation was in progress. Hydrogen-air mixture was programmed as Cantera „gas"object and calculations, according to both Mevel2017 and ZND algorithms, were performed directly on it.

4 Results

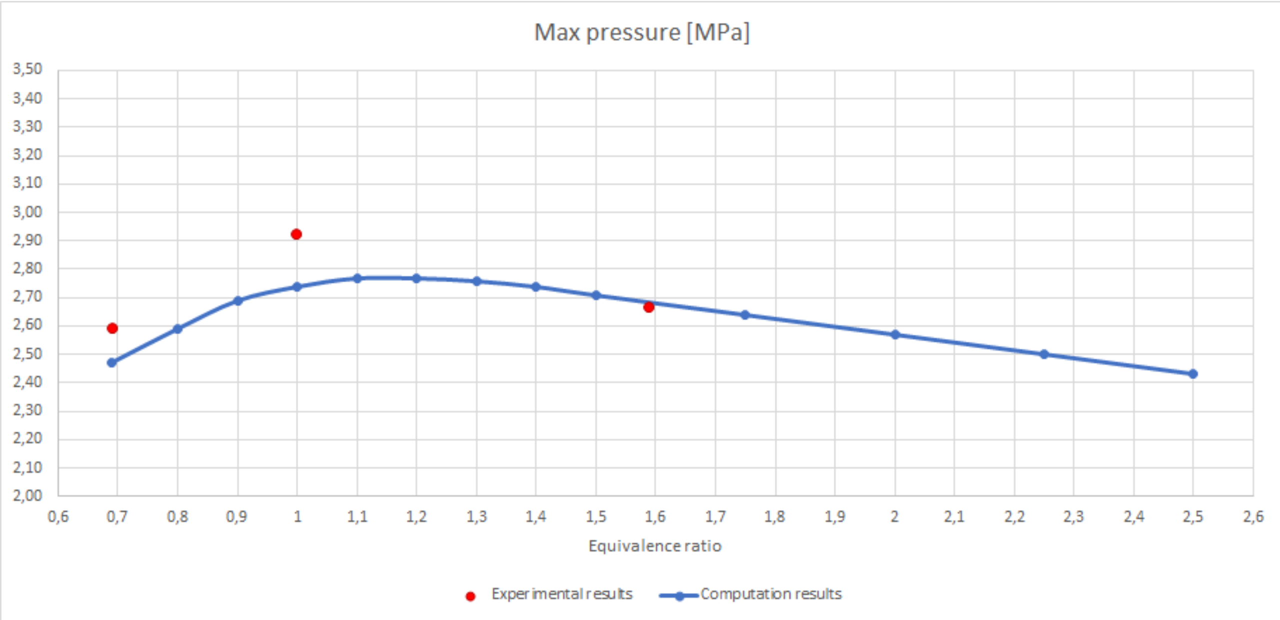

Figure 1: The maximum pressure.

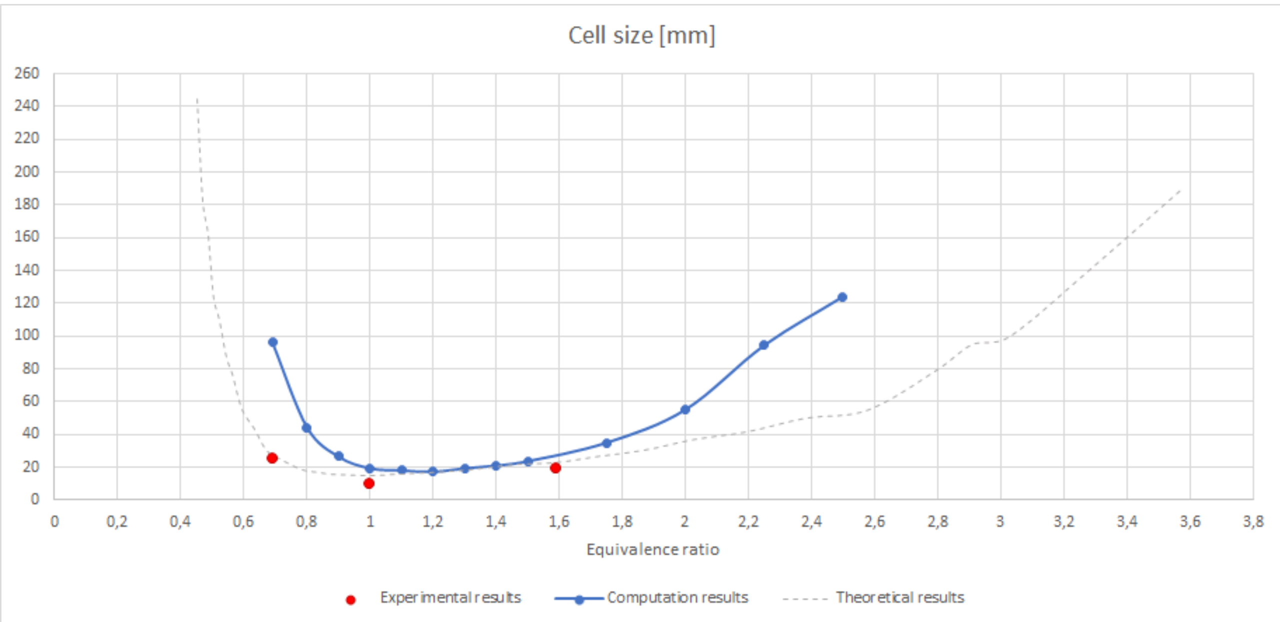

Figure 2: The cell size.

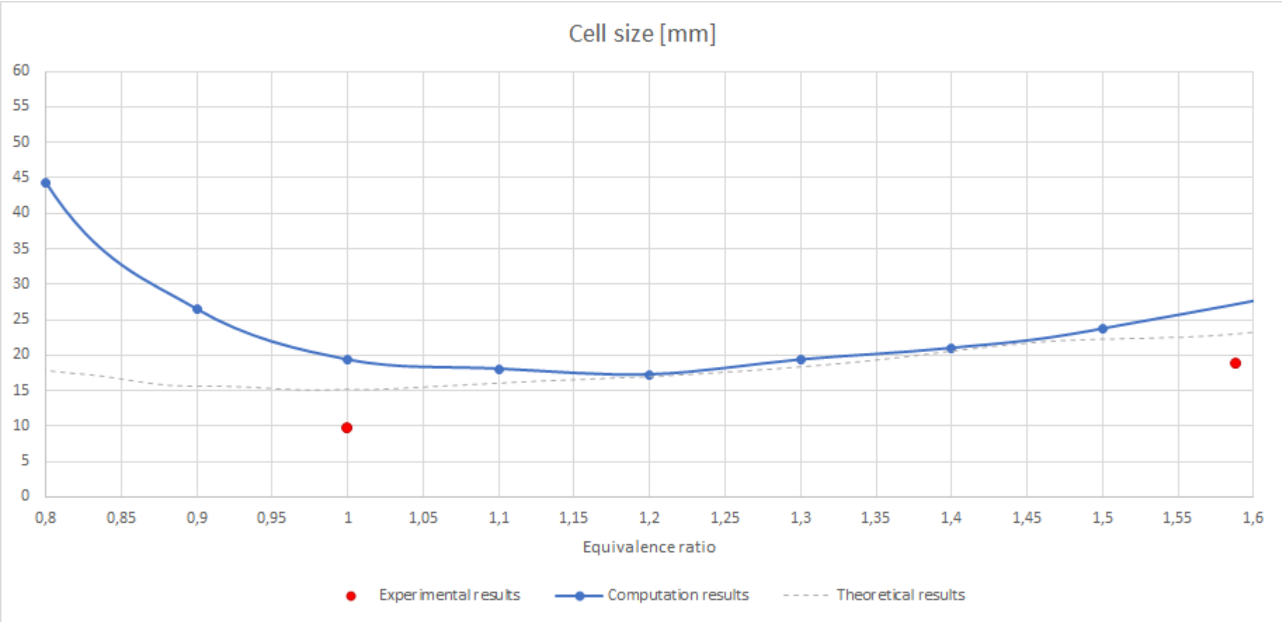

Figure 3: The cell size in details.

5 Summary

Computed results match with experimental data shows slight discrepancies both in maximum pressure and cell size prediction. Good convergence was achieved in a vicinity of equivalence ratio equal to 1.6, however prediction seems to be reasonable as maximum pressure was predicted to peak and cell size to reach global minimum for stoichiometric mixtures.

References

[1] Max pressure: *sdtoolbox.githut.io*;

[2] Cell size: *sdtoolbox.githut.io*;

[3] Model of ZND: *sdtoolbox.githut.io*;

[4] Theoretical and experimental data: Laboratory of combustion;