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# NUMERICAL AND EXPERIMENTAL INVESTIGATION OF METHANE-OXYGEN DETONATION IN A 9 M LONG TUBE

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***Abstract***

*Numerical investigation of methane-oxygen detonation parameters was conducted with an OpenFoam code. Custom solver ddtFoam made especially for detonation problems was made use of. It uses the HLLC scheme to resolve the discontinuities and the subgridscale model to improve results on coarse meshes. Combustion model is based on progress variable equation, which contains two source terms. The first is the deflagrative source term and is modelled using the Weller correlation. The second is the detonative source term and it accounts for autoignition effects. Range of analysed gaseous mixture compositions was 20, 33 and 40% of methane in oxygen. The 2D calculation geometry was a 9 m long pipe with diameter 0.17 m. The mesh consisted of 382 500 hexahedral cells with the dimensions of 2x2 mm. Experimental results such as pressure profiles and detonation velocities are presented. Simulations were performed using LES turbulence model (k-equation-eddy-viscosity model) and compared with experimental data. Various dynamic parameters, like for example reaction lengths for methane-oxygen detonations, are estimated from the steady ZND analyses conducted in Cantera and SDToolbox libraries and based on GRI 3.0 kinetic mechanism of methane combustion. These lengths were then used in empirical formulas to obtain the characteristic cell sizes and assessed against experimental data.*

***Keywords:*** *detonation, methane, combustion, simulation, experiments, characteristic cell size*

## 1. Introduction

Detonation is the most dangerous type of combustion where a supersonic wave, which is also a flame front, propagates through a fresh mixture increasing pressure and temperature. Due to the exponential dependency of the chemical reaction rate on temperature [5] intense combustion occurs, which continuously supports the shock [6]. The propagation speed in detonations of gaseous mixtures varies from 1000 to 3500 m/s. The reaction zone length for the most of stoichiometric fuel-air mixtures is less than 10 mm. For fuel-oxygen mixtures, it is less than 0.1 mm [1].

A detonation wave is in fact a multi-dimensional structure. It consists of Mach stems, incident shocks and transverse waves, which interact with each other and form triple points. These create detonation cells. Their size depends mostly on the mixture composition. The Zeldovich, von Neumann and Döring (ZND) theory implies that the detonation wave consists of a shockwave, and a reaction zone, which end is defined by the Chapman-Jouguet (CJ) condition (M = 1) [3]. The

ZND reaction length is used for example in empirical calculations of the detonation characteristic cell sizes [6].

The aim of this study was to validate the methane-oxygen mixture detonation parameters obtained in simulations against the experiments performed in the 9 m long tube with the diameter of 0.17 m.

## 2. Experiments and setup

Experiments were conducted in a 9 m long tube with 0.17 m of inner diameter. Analysis concerned mixtures of 20, 33 and 40% vol. of methane in oxygen. The initiation of detonation took place in a 0.6 m long turbulence generator. It consisted of metal layers, which created a mesh just behind the spark plug located at the beginning of the tube. The mixture was ignited with that spark plug and detonation was initiated on a distance of 0.5 m from the ignition point. The aim of these experiments was to obtain pressure profiles and characteristic cell sizes. Pressure as a function of time was measured by nine piezoelectric sensors and flame occurrence was determined by nine photodiodes. The first pair of sensors was placed 0.5 m from the ignition point and the rest of them every 1 m. Metal sheets were covered with soot and placed at the end of the detonation pipe. After the detonation, characteristic cell sizes were measured by a calliper on a metal sheet multiple times and then the mean value was determined. Mixtures used for analysis were prepared in cylinders using the partial pressures method and stored horizontally for no longer than 24 hours. Absolute initial pressure of mixtures in every experiment was equal to 1 bar and temperature was 25°C.

## 3. Solver and modelling

Numerical simulations were conducted in OpenFoam software. Calculations were performed for Large Eddy Simulation (LES) k-equation eddy-viscosity model turbulence model [11].

ddtFoam solver was created by Ettner et al. [2]. It solves the unsteady and compressible Navier-Stokes equations based on density. All convective terms are solved with the use of HLLC scheme [9] with multidimensional limiter [12], which allows for more accurate representation of shock waves than for example standard PISO scheme. Combustion is described by a progress variable $c$, which takes values: $c = 1$ – completely burned mixture, $c = 0$ – unburned mixture. Transport equation of c variable is as follows:

$$\frac{\partial}{\partial t}(\overline{\rho}\widetilde{c}) + \frac{\partial}{\partial x_j}(\overline{\rho}\,\widetilde{c}\,\widetilde{u}_j) = \frac{\partial}{\partial x_j}(\overline{\rho} D_{eff}\,\frac{\partial \widetilde{c}}{\partial x_j}) + \overline{\omega}_{c,def} + \overline{\omega}_{c,ign}\,, \tag{1}$$

where:

$x_j$ – j-th direction coordinate,
$u_j$ – j-th velocity coordinate,
$t$ – time,
$\overline{\rho}$ – Reynolds-averaged density,
$\widetilde{c}$ – Favre-averaged combustion progress variable,
$D_{eff}$ – effective dissipation coefficient,
$\overline{\omega}_{c,def}$ – deflagrative source term,
$\overline{\omega}_{c,ign}$ – detonative source term.

The deflagration source term is based on the Weller model with flame quenching [10]. Source term for detonation is based on autoignition effects, where the autoignition delay is precalculated using Cantera code [14] with the GRI 3.0 mechanism [13] and placed in a table.

Subgrid-scale model takes into account the possibility that the conditions of self-ignition can occur in a cell even if the shock wave have not travelled past it yet. This situation can cause

remarkable errors in the results, especially in coarser grids. Model used in this solver introduces the $\alpha$ parameter, which virtually divides cells into high and low pressure and temperature zones. It allows igniting only that section of a cell, which really satisfies conditions for self-ignition.

## 4. Numerical model

A 2D rectangular geometry with dimensions of 9000 mm x 170 mm was used in the simulations. Generated mesh was orthogonal and structural. It contained 382 500 hexahedral cells. LES k-equation eddy-viscosity model was used for turbulence modelling [11]. Simulations were conducted for 20, 33 and 40% of methane in oxygen, because the experiments showed that detonation occurs in these limits, and then compared with experiments.

## 5. Cell size calculations

Reaction length was calculated using ZND code for SDToolbox [15] based on GRI 3.0 mechanism [13]. Three definitions, suggested in the work of Shepherd [6], were used to calculate reaction length. Reaction length is defined as a distance from von Neumann's peak to:

– M = 0.9 indicated as $\Delta_1$,
– M = 0.75 indicated as $\Delta_2$,
– $(\mathrm{d}T/\mathrm{d}x)_{\max}$ (induction length) indicated as. $\Delta_3$.

In order to calculate the characteristic cell sizes the following empirical equation was used:

$$\lambda_i = 29 \cdot \Delta_i \,, \tag{2}$$

where $\lambda_i$, ($i$ = 1, 2 and 3) are the respective cell sizes defined based on $\Delta_1$, $\Delta_2$ and $\Delta_3$ reaction length definitions. Constant coefficient was selected based on [7].

## 6. Experimental results

Data acquired from sensors was analysed and shown on the following pressure plots: Fig. 1, 2 and 3. The numbers on a horizontal axis on velocity plot (Fig. 4) stand for the middle points between every two sensors. Pressures above 30 bar and velocities larger than 2000 m/s for 20, 33 and 40% show that detonation occurs for these concentrations.

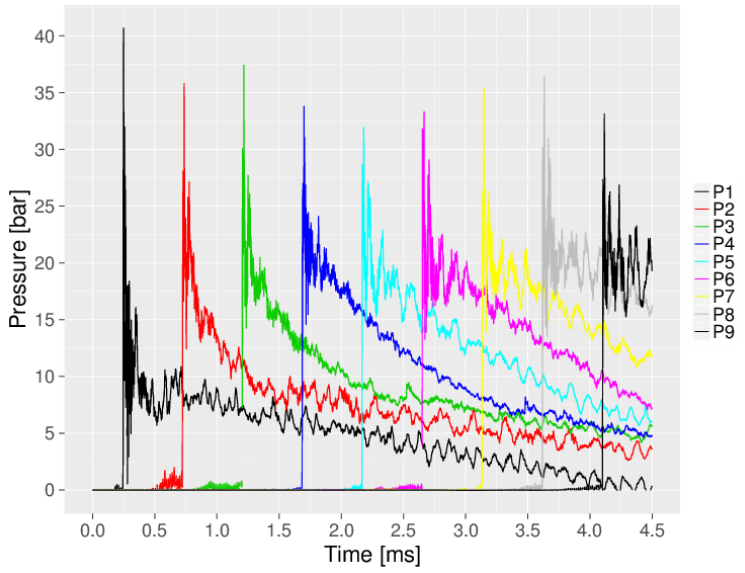


*Fig. 1. Pressure distribution measured for 20% of methane in oxygen*

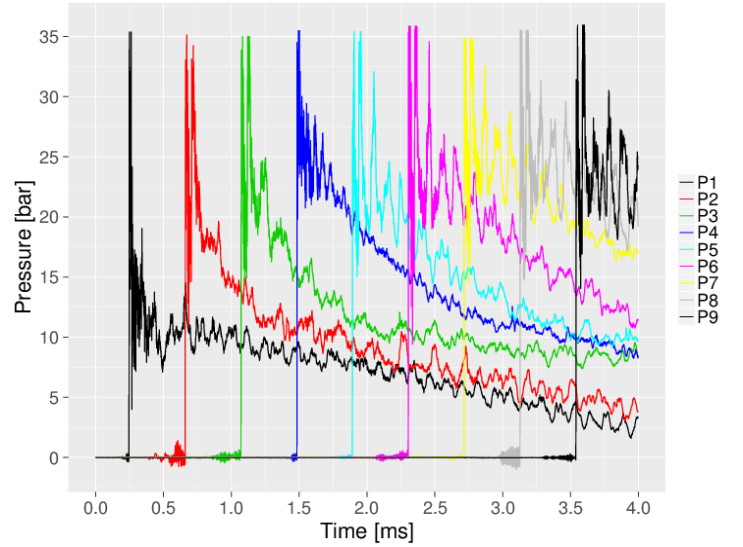


*Fig. 2. Pressure distribution measured for 33% of methane in oxygen*

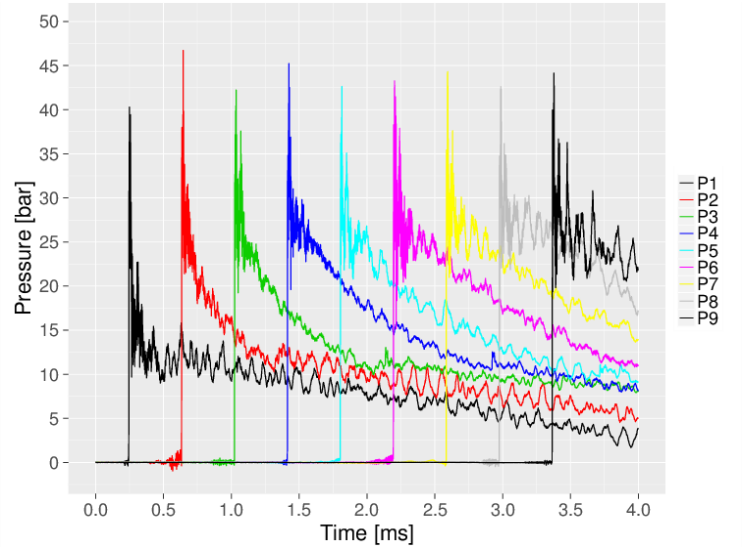


*Fig. 3. Pressure distribution measured for 40% of methane in oxygen*

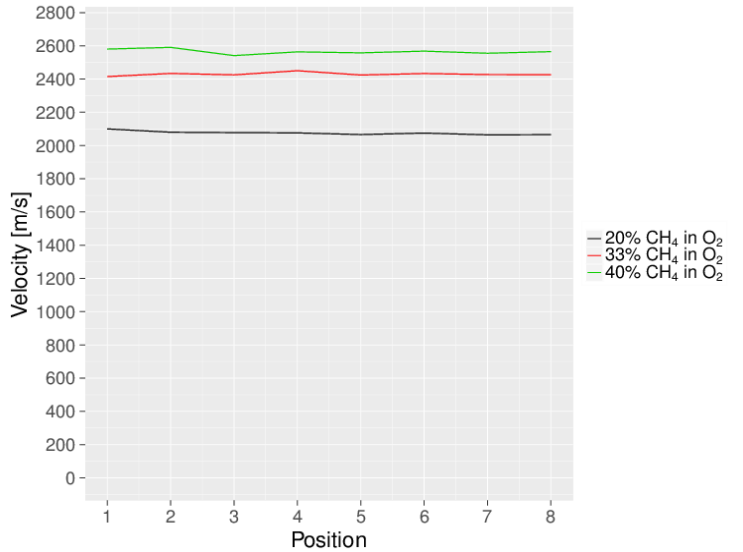


*Fig. 4. Flame propagation velocity obtained in experiments*

## 7. Comparison of experiments and simulations

Pressure profiles and detonation velocities obtained in simulations were compared with experimental results. Pressure plots are shown on Fig. 5, 6 and 7. The shock wave in simulations was faster by about 0.2 to 0.25 ms and pressure peaks were mostly larger in simulations generally by a range of values from 2 to 10 bar and up to 22 bar in a few occurrences. Velocity plots are shown on Fig. 8. Simulations produced values larger by about 100 m/s to 150 m/s, while for 20% concentration the error was the smallest.

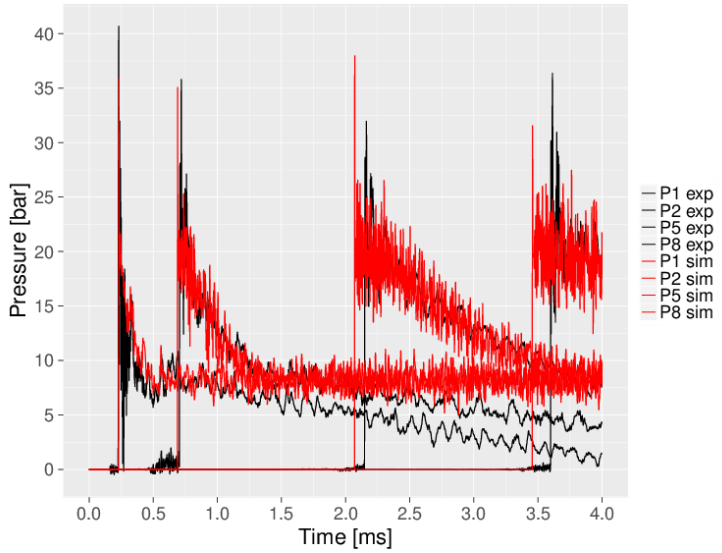


*Fig. 5. Comparison of pressure from simulation and experiment for 20% of methane in oxygen*

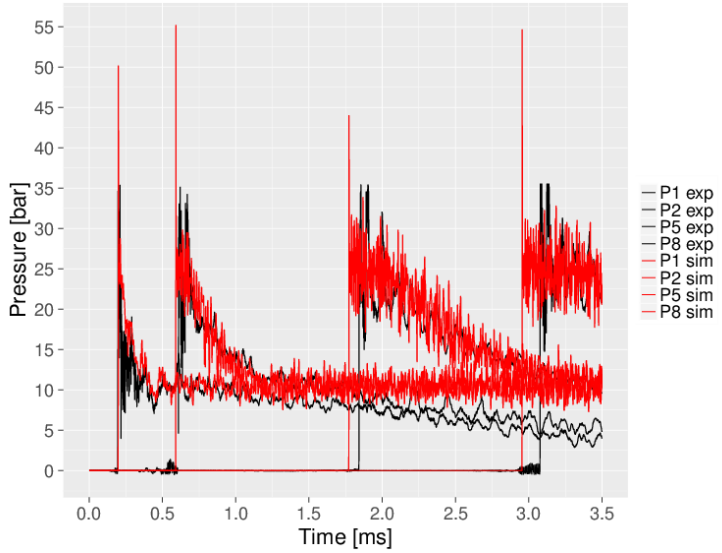


*Fig. 6. Comparison of pressure from simulation and experiment for 33% of methane in oxygen*

## 8. Cell sizes – experiments

During the experiments characteristic cell sizes were measured several times in order to take the average value for every concentration. These averages were shown on the figure 9 for 20, 33 and 40% of methane in oxygen. It can be noticed that the smallest cell size appeared for the stoichiometric methane-oxygen mixture (~33%) and was equal to 2.9 mm. However, other experiments [8] showed that smaller cells appear slightly above the stoichiometric concentrations.

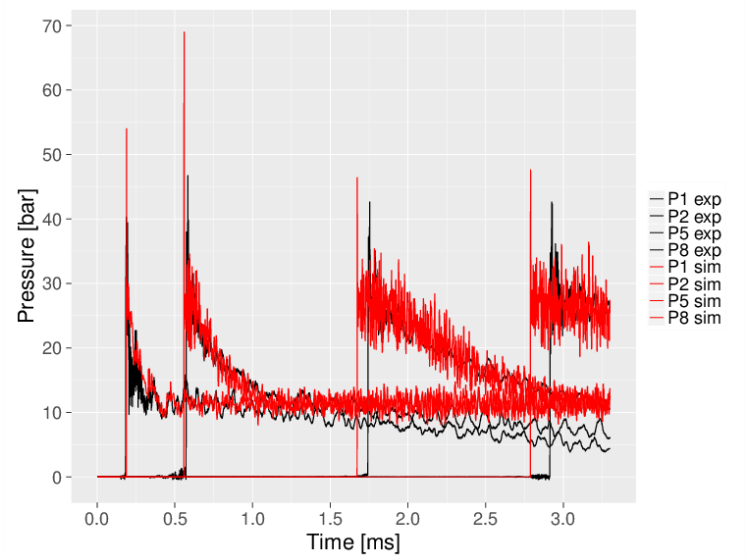


*Fig. 7. Comparison of pressure from simulation and experiment for 40% of methane in oxygen*

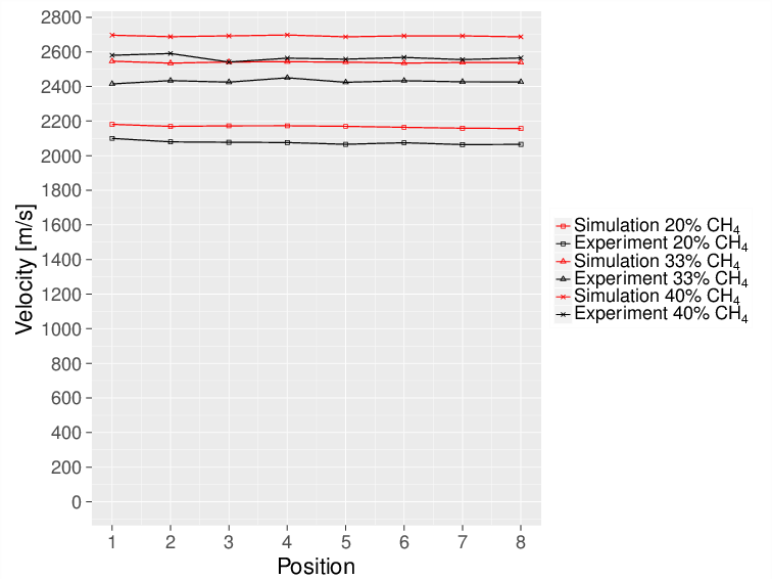


*Fig. 8. Comparison of velocity from simulations and experiments*

## 9. Cell sizes – computations and comparison

Calculations of the ZND reaction lengths were conducted. Results are shown in Tab. 1. Next, using equation (2) the respective cell sizes were obtained. Then, they are shown and compared with experiments on Fig. 9. It shows that the best results, for the coefficient chosen as in eq. (2), were obtained for the $\Delta_2$ and $\Delta_3$ definitions of the reaction length. They are the most accurate for the 40% concentration and do not differ from the experiments. The biggest error occurred for 20% of methane where the calculation result was lower by over 7.5 mm, which gave the relative error of almost 100%. The same was for the stoichiometric concentration. The difference was 3 mm and the relative error was equal to 100%.

## 10. Conclusions

In this study the experimental and numerical investigation on parameters of methane-oxygen detonations was performed.

*Tab. 1. Calculated ZND reaction lengths*

| | $\Delta_1$ [mm] | $\Delta_2$ [mm] | $\Delta_3$ [mm] |
|---|---|---|---|
| 20% $CH_4$ | 0.72794 | 0.54932 | 0.52849 |
| 33% $CH_4$ | 0.29798 | 0.20752 | 0.20060 |
| 40% $CH_4$ | 0.26749 | 0.17448 | 0.16560 |

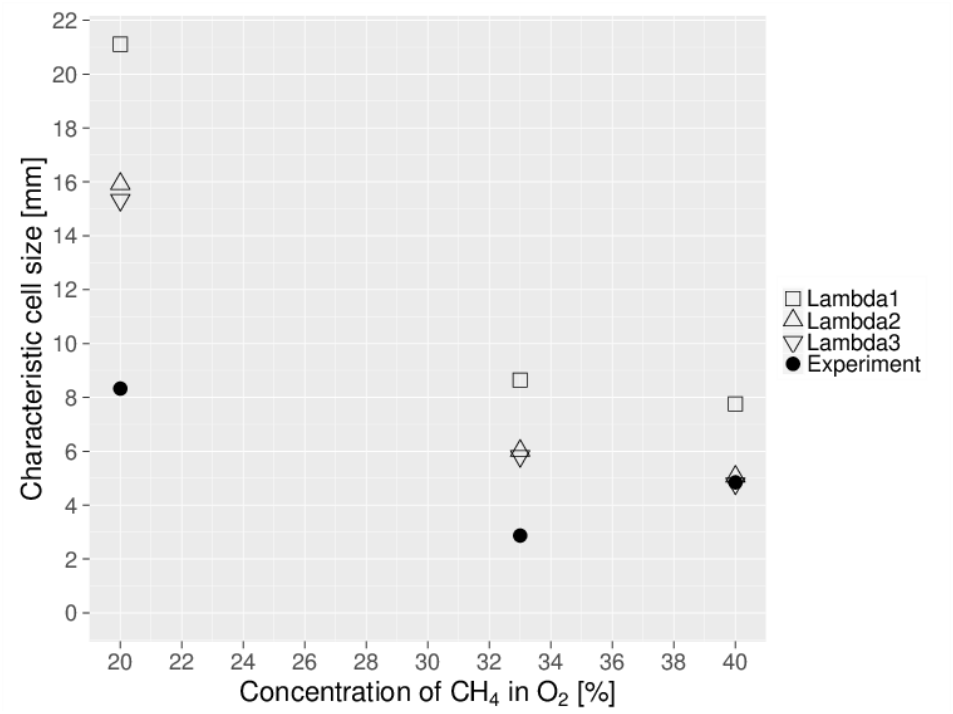


*Fig. 9. Comparison of characteristic cell sizes from calculations and experiments*

The comparison between simulations showed that ddtFoam overestimated every velocity by values from 100 m/s to 150 m/. Pressures from simulations were generally too large. Their values differed from 2 to 10 bar with a few exceptions as of 22 bar. It can be concluded, that while pressure values and errors varied for every concentration and even for every sensor, velocities were predicted rather well and obtained errors were similar for every concentration.

Computations of characteristic cell sizes using the selected empirical formula (2), gave accurate results only for 40% concentration and for $\Delta_2$ and $\Delta_3$ definitions of the reaction length. For the rest of the concentrations the relative errors were close to 100%, which is too large. It was said in [7], that standard empirical formulas could give good approximations of the characteristic cell based on the reaction lengths only for a few concentrations, generally close to the stoichiometric. These computations showed that even for stoichiometric concentrations the empirical formulas could give large errors. Generally, the linear, empirical correlation depends heavily on the chosen definition of the reaction length and on the given fuel. In addition, it cannot be used for a wide range of concentrations. More advanced non-linear correlations [4] should be used instead.

## Acknowledgments

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