NUMERICAL AND EXPERIMENTAL INVESTIGATION OF H2-AIR AND H2-O2 DETONATION PARAMETERS IN A 9 M LONG TUBE, INTRODUCTION OF A NEW DETONATION MODEL

Malik K.[1], Żbikowski M.[1], Bąk D.[2], Lesiak P.[2] and Teodorczyk A.[1]
[1] Institute of Heat Engineering, Warsaw University of Technology, Nowowiejska 21/25, 00-665 Warsaw, Poland, konrad.malik@gmail.com
[2] Scientific and Research Centre for Fire Protection National Research Institute, Aleja Nadwiślańska 213, 05-420 Józefów, Poland, plesiak@cnbop.pl

ABSTRACT

Experimental and numerical investigation of hydrogen-air and hydrogen-oxygen detonation parameters were performed. A new detonation model was introduced and validated against the experimental data. Experimental set-up consists of 9 m long tube with 0.17 m in diameter, where pressure was measured with piezoelectric transducers located along the channel. Numerical simulations were performed within OpenFoam code based on progress variable equation where the detonative source term accounts for autoignition effects. Autoignition delay times were computed at a simulation run-time with the use of a multivariate regression model, where independent variables are: pressure, temperature and fuel concentration, dependent variable: autoignition delay time. Range of the analysed gaseous mixture composition varied between 20% to 50% of hydrogen-air and 50% to 66% of hydrogen in oxygen. Simulations were performed using LES one-equation eddy viscosity turbulence model in 2D and 3D. Calculations were validated against experimental data.

1.0 INTRODUCTION

Detonation is a dangerous combustion regime. In this phenomenon, a supersonic wave (coupled reaction front with leading shock wave) propagates through a fresh mixture. Pressure and temperature can rise significantly across detonation wave. The speed of the propagating detonation directly depends on the compression rate across the wave, while rapid energy release supports the detonation. Typical propagation velocities of detonations vary between 2500 to 7000 m/s [1]. The reaction zone length for fuel-air mixtures is usually less than 10 mm, while for fuel-oxygen it is less than 0.1 mm [2]. In many risk assessments, only deflagration is considered as a most probable scenario. However, detonation is a menace, taking into consideration the fact, that hydrogen detonation limits are very wide (18.3% to 59% for hydrogen-air, 15% to 90% for hydrogen-oxygen). The structure of a detonation wave is multi-dimensional, where Mach stems, transverse waves and incident shocks collide with each other forming triple points and creating detonation cells. The size of the cells depends on the mixture composition. The Zeldovich, von Neumann and Döring (ZND) theory states, that the detonation wave is one-dimensional and consists of a precursor shock and a combustion zone. Fresh mixture is compressed adiabatically by von Neumann shock wave. It reaches the autoignition temperature and reacts in the reaction zone, which follows immediately after the shock ends when the Chapman-Jouguet condition is reached (Mach number M = 1) [3]. Detonation wave thickness is a distance from the beginning of the shock wave to the end of the reaction zone. Behind the reaction zone, the pressure drops down in the expansion fan. This expansion pushes the combustion products away from the detonation, which produces a force which supports propagation of the detonation wave. One-dimensional form of detonation is not observed in experiments. Instead, it is a three-dimensional and unstable structure. Nevertheless, models based on the ZND theory are frequently used to validate detailed chemical mechanisms. The reaction length defined by the ZND theory often finds its use in calculations of the detonation characteristic cell sizes [4].

In this work an experimental investigation of hydrogen – air and hydrogen – oxygen detonation in a 9 m long tube with inner diameter 0.17 m is presented. The main aim of this work was to introduce a

new detonation model and describe measured distribution of the detonation cell size for wide range of hydrogen – oxidant composition.

2.0 EXPERIMENTS AND SETUP

Experiments were conducted in a 9 m long detonation tube with 0.17 m of inner diameter. The combustion was initiated with the use of a spark plug located at the beginning of a 0.6 m long turbulence generator (made of multiple layers of metal mesh), where the transition to detonation were taking place (approximately 0.5 m from the ignition point for all mixtures). The purpose of the experiments was to acquire pressure profiles, detonation velocity and the distribution of the characteristic cell sizes for specific mixture composition. Nine piezoelectric sensors were used to measure pressure. The flame occurrence was tracked with nine photodiodes. Pressure sensors and photodiodes were placed in pairs. The first pair 0.5 m from the beginning of the tube, and every next pair at respectively: 1.5 m, 2.5 m, 3.5 m, 4.5 m, 5.5 m, 6.5 m, 7.5 m and 8.5 m. In order to measure the characteristic cell sizes, a metal sheet covered with soot was used. It was placed at the end of the tube, and the cells were measured with a caliper. All mixtures were prepared using the partial pressures method the day before the experiment. Experiments were conducted under pressure of 1 bar and the temperature 25°C. Mixtures in the range of 15 to 60% of hydrogen in air and 15 to 90% of hydrogen in oxygen were investigated. In this work only selected concentrations are presented.

3.0 NUMERICAL ANALYSIS AND MODELING

3.1 Solver

Numerical simulations were conducted in OpenFoam 2.1.1 [5] software using ddtFoam solver and Large Eddy Simulation (LES) turbulence model [6]. The ddtFoam library [7] solves the unsteady and compressible Navier-Stokes equations density based. Convective terms are solved using the HLLC Riemann scheme [8] with multidimensional limiter [5], which allows for more accurate capturing of discontinuities than standard schemes. Combustion is characterized by a progress variable c, where: c = 1 - burned mixture, c = 0 - unburned mixture. The transport equation of c is as follows:

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{c})+\frac{\partial}{\partial x_j}(\bar{\rho}\tilde{c}\tilde{u}_j)=\frac{\partial}{\partial x_j}(\bar{\rho}D_{eff}\frac{\partial \tilde{c}}{\partial x_j})+\bar{\omega}_{c,\mathrm{def}}+\bar{\omega}_{c,\mathrm{ign}}, \quad (1)$$

where: c - combustion progress variable; D_{eff} – effective diffusion coefficient; ρ – density; $\omega_{c,def}$, $\omega_{c,ign}$ - deflagration and detonation source terms; u_j - j-th element of velocity; x_j – j-th space coordinate; ¯ - Reynolds averaging; ~ - Favre averaging.

The right hand side of the equation (1) presents two source terms which account respectively for deflagration and detonation. The deflagration source term is based on the Weller deflagration model with an additional flame quenching [9]. The detonation source term is based on the model of autoignition delay time described in the section 3.3.

3.2 Numerical model

Numerical investigation was conducted within two calculation domains: 2D and 3D. The 2D geometry had the dimensions of 9 m x 0.170 m. Mesh was orthogonal and structural, and contained 382 500 hexahedral cells. The 3D mesh consisted of 2 520 000 hexahedral cells with an average dimensions of about 4.5x4.5x4.5 mm. Simulations were conducted for 20%, 30% and 50% of hydrogen in air, as well as 50% and 66% of hydrogen in oxygen. 3D simulations were performed only for stoichiometric concentrations of hydrogen-air (30%), and hydrogen-oxygen (66%) mixtures in order to verify results. Numerical simulations were validated against experimental data.

3.3 Ignition time delay model

Ignition delay time model is based on multivariate regression analysis [10,11]. Data for model training was obtained using Cantera code [12] with the h2air_highT [13] (hydrogen-air) and h2o2_highT mechanism [14] (hydrogen-oxygen), which are the derivatives from the GRI30 mechanism [15]. This mechanism showed good agreement with experimentally obtained ignition delay times of hydrogen-air and hydrogen-oxygen mixtures [16,17]. The following quantities were chosen as independent variables: p – pressure, Tu – temperature of the unburned mixture, fH – unburned hydrogen mass fraction. The ranges of these parameters used for data generation were as follows: pressure 0.1-150 bar, temperature 800-4500 K, hydrogen volumetric fraction 4%-75% (H_2-air) and 4%-94% (H_2-O_2). These features produced two matrices with approximately 16 000 rows. The dependent variable was $\log(t_{ign})$ – the logarithm of the autoignition delay time. In the regression 2nd, 3rd and 4th degree polynomials were used. A five-fold cross-validation was done in order to obtain the best results, independent of the selection of train and test data. After the analysis, the 3rd degree polynomial was chosen to give the best results. The following formula (2) was used:

$$\begin{aligned}\log(t_{ign}) = {} & C_0 + C_1\cdot fH + C_2\cdot fH^2 + C_3\cdot fH^3 + C_4\cdot p + C_5\cdot p^2 + C_6\cdot p^3 + C_7\cdot Tu + C_8\cdot Tu^2 + C_9\cdot Tu^3 \\ & + C_{10}\cdot fH\cdot p + C_{11}\cdot fH\cdot Tu + C_{12}\cdot p\cdot Tu + C_{13}\cdot fH^2\cdot p + C_{14}\cdot fH^2\cdot Tu + C_{15}\cdot p^2\cdot fH + C_{16}\cdot p^2\cdot Tu \\ & + C_{17}\cdot Tu^2\cdot fH + C_{18}\cdot Tu^2\cdot p + C_{19}\cdot fH\cdot p\cdot Tu\end{aligned}, \qquad (2)$$

where the parameters for both mixtures are presented in the table 1. The r-squared parameter for the both formulas was around 0.88.

Table 1. Coefficients of the regression equation

Coefficient	Hydrogen - air	Hydrogen - oxygen
C_0	5.683	6.311
C_1	1.594	-11.675
C_2	16.645	22.452
C_3	-55.85	-13.595
C_4	-2.667e-07	-1.773-07
C_5	4.189e-14	4.565e-14
C_6	-1.113e-21	-1.326e-21
C_7	-1.137e-02	-1.23e-02
C_8	3.603e-06	3.923e-06
C_9	-3.975e-10	-4.306e-10
C_{10}	-1.714e-07	-3.134e-07
C_{11}	-1.194e-03	5.69e-03
C_{12}	-1.142e-10	-1.865e-10
C_{13}	3.42e-07	3.001e-07
C_{14}	-6.158e-04	-4.66e-03
C_{15}	-5.549e-15	2.211e-15
C_{16}	-4.119e-18	-3.716e-18
C_{17}	5.387e-08	-6.205e-07
C_{18}	3.658e-14	4.726e-14
C_{19}	7.994e-11	4.196e-11

4.0 RESULTS AND DISCUSSION

4.1 Experiments

Data gathered from the experiments were postprocessed and presented in fig. 1 for hydrogen-air (20% and 30% concentrations), and fig. 2 for hydrogen-oxygen mixtures (50% and 66% concentrations). Pressure varied between 20 - 40 bar for the hydrogen-air mixtures, with one exception for the 30% mixture in fig. 1, where pressure rose above 50 bar. For hydrogen-oxygen mixtures it was 20 to 30 bar with one exception of approx. 34 bar. Measured velocities for hydrogen-air and hydrogen-oxygen mixtures are compared with the theoretical Chapman-Jouguet [4] velocity (computed using SDToolbox [18]) in fig. 3. It can be seen, that the velocities for both mixtures were very close to the CJ speed (+/- 20 m/s). Characteristic cell sizes for both mixtures are presented in fig. 4. The measurements were done using slide caliper with a $5 \cdot 10^{-4}$ m accuracy. For each concentration of hydrogen in both mixtures 100 readings were done. Boxes represent quartiles (25%) of the data (second and third quartile). Middle line shows the mean value. Lines extending vertically from the boxes (whiskers) indicate variability outside the upper and lower quartiles. It can be seen that detonation cells have normal distribution, but in each case some outliers are present (black dots). It can be noticed, that the characteristic cell sizes for H_2-O_2 mixtures are one order of magnitude smaller. It means that this mixture is much more reactive. Moreover, it can be noticed, that the measured values for concentrations that are farther from stoichiometry (20%, 50% for H_2-air and 50% for H_2-O_2) have larger boxes. For these mixtures, measured cells varied in size and had irregular structure.

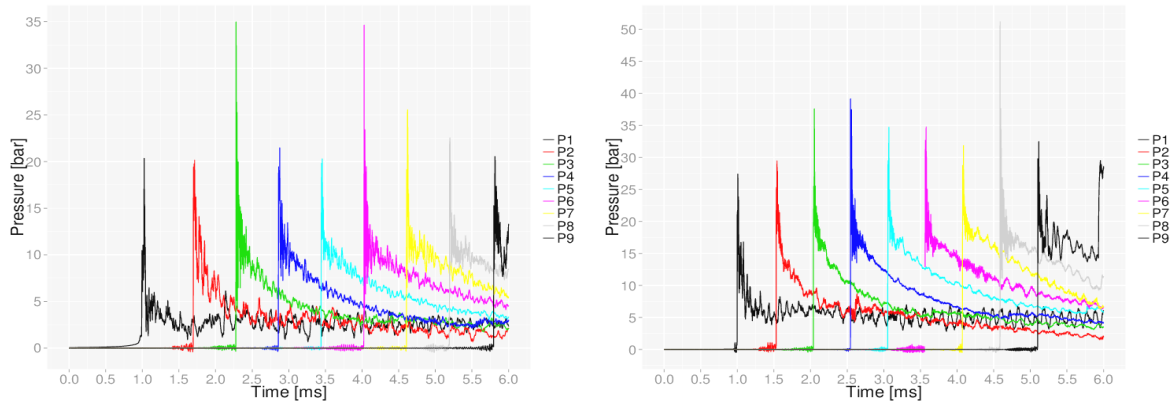
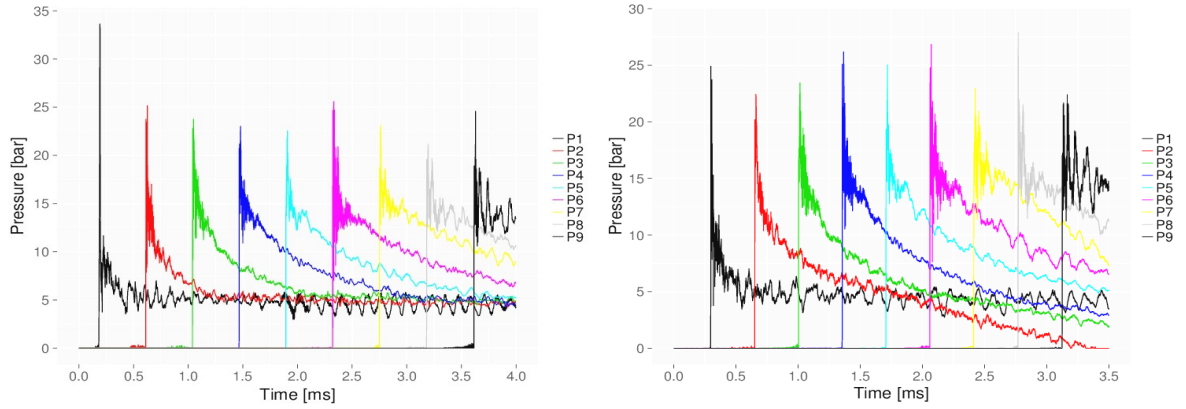
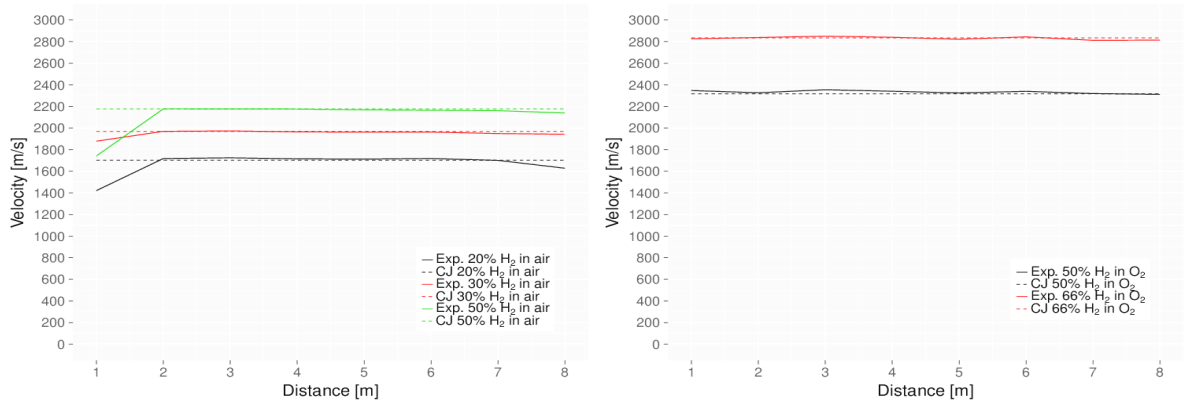


Figure 1. Pressure distribution measured for 20% (a) and 30% (b) of hydrogen in air



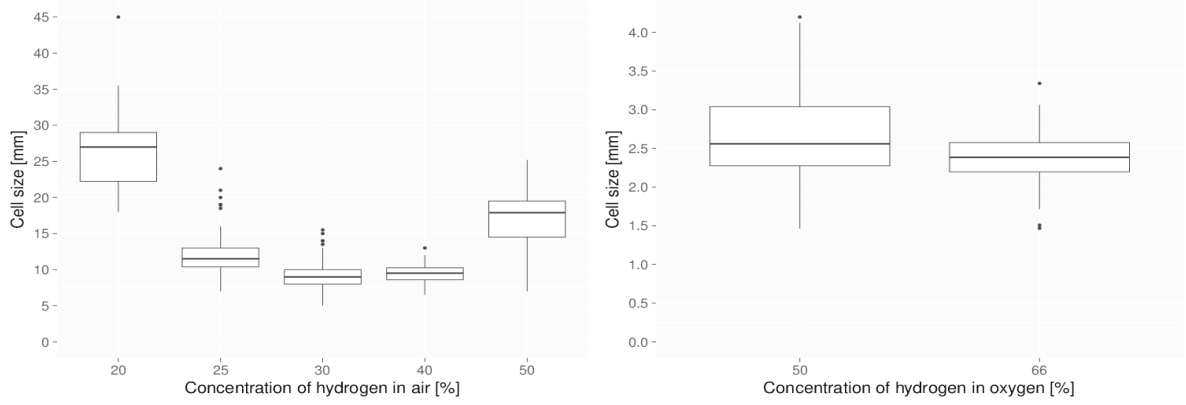
(a) (b)

Figure 2. Pressure distribution measured for 50% (a) and 66% (b) of hydrogen in oxygen



(a) (b)

Figure 3. Flame propagation velocity obtained in experiments. (a) H_2-air mixture, (b) H_2-O_2 mixture



(a) (b)

Figure 4. Characteristic cell sizes obtained in experiments: (a) H_2-air mixture, (b) H_2-O_2 mixture

4.2 Results of numerical simulation

Results obtained from simulations using the new detonation model were compared with the experimental results. Pressure comparisons for 20% and 30% hydrogen-air mixtures with 2D simulations were shown in fig. 5. For 50% and 66% hydrogen-oxygen mixture it was fig. 6. It can be seen that the results are in good agreement with experimental data. The detonation in simulations is ahead of measurements 0.2 to 0.3 ms. Moreover, maximum pressure peaks obtained in calculations were underresolved by values from 1 to 10 bar. Results from 3D simulations were gathered and compared in fig. 7. Pressure values were smaller in 3D simulations compared to 2D. Velocity plots are shown in figure 8 for hydrogen-air and hydrogen-oxygen respectively. Simulation gave values close to the experimental measurements. Velocities were overpredicted by approximately 100 m/s, with an exception for 20% of hydrogen in air, where difference is close to 50 m/s. For 66% of hydrogen in oxygen, where it was about 150 m/s. In the 3D case of 66% H_2-O_2 mixture the simulation was 50-100 m/s faster, than 2D. This difference is caused by the fact that the mesh for 3D case was too coarse. For 30% of hydrogen in air, the 3D simulation gave velocity which was the same as in 2D with an accuracy of up to 5 m/s.

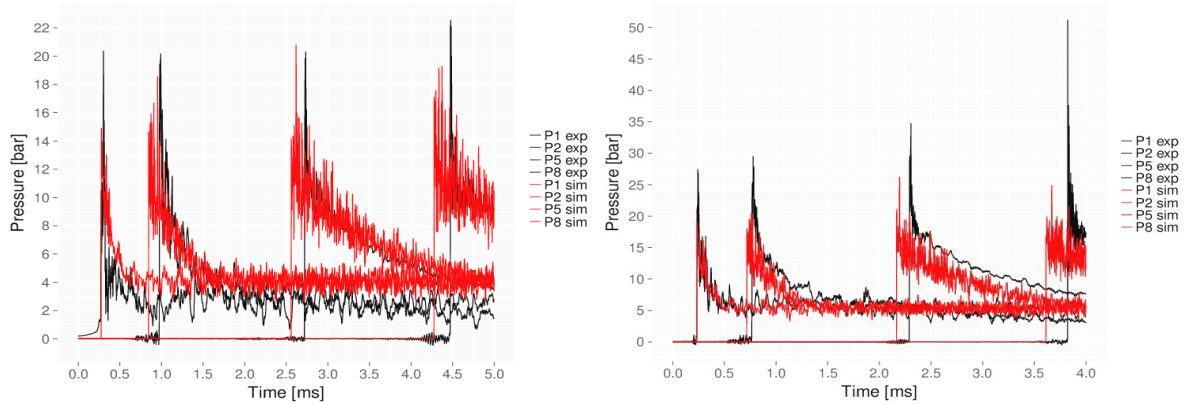


Figure 5. Pressure comparison from 2D simulation and experiment: (a) 20% and (b) 30% of H_2 in air

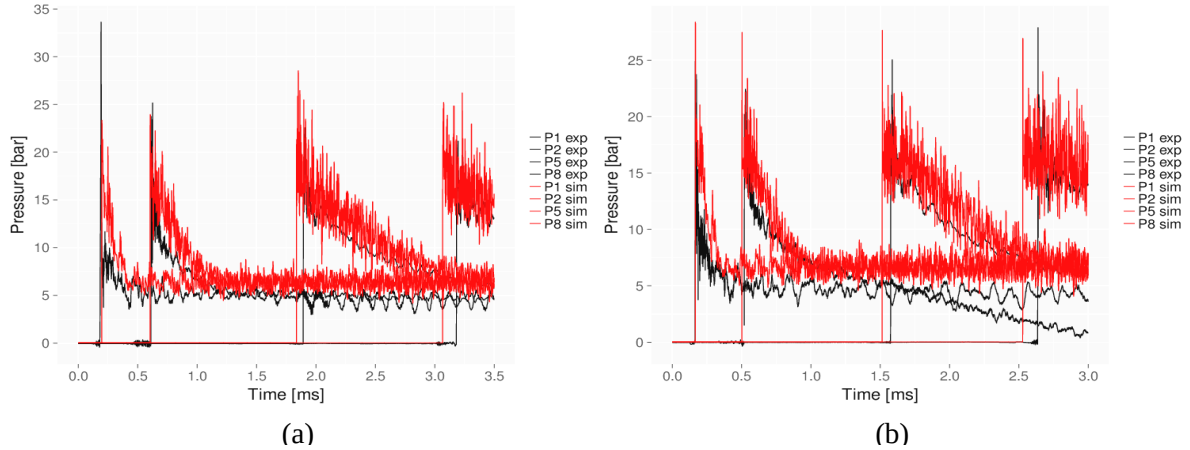


Figure 6. Pressure comparison from 2D simulation and experiment: (a) 50% and (b) 66% of H_2 in O_2

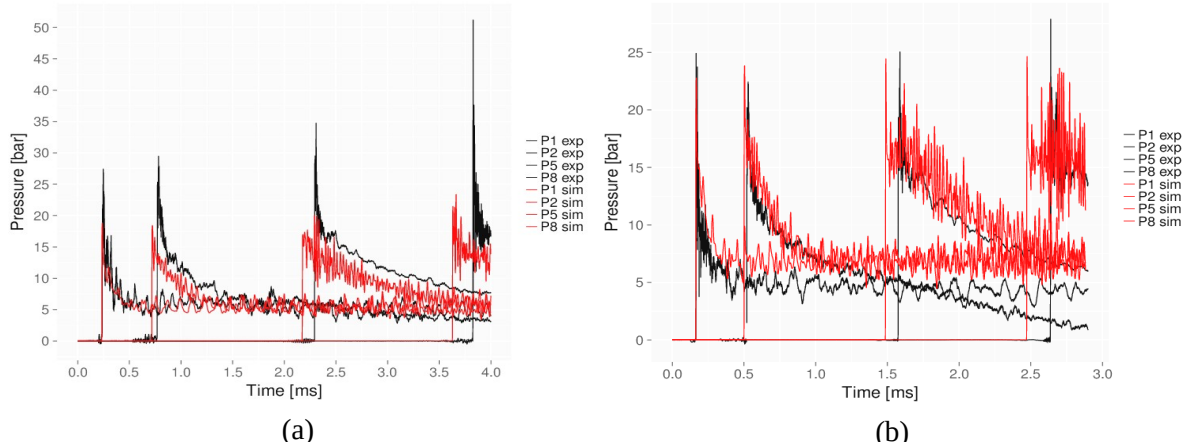


Figure 7. Pressure comparison from 3D simulation and experiment: (a) 30% H_2 in air and (b) 66% of H_2 in O_2

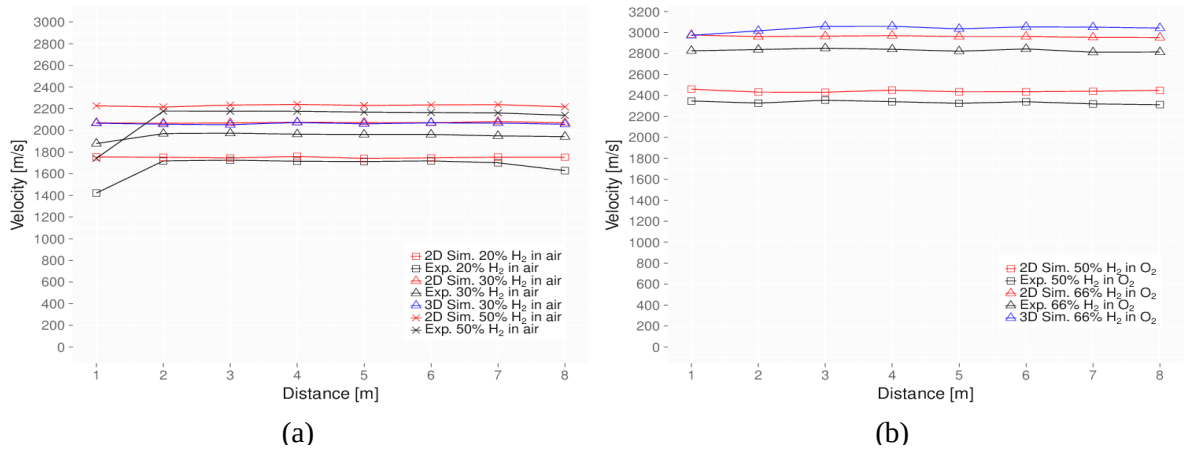


Figure 8. Velocity comparison from 3D simulation and experiment: (a) H_2-air, (b) H_2-O_2

5.0 CONCLUSIONS

In this study the experimental and numerical investigation of hydrogen-air and hydrogen-oxygen detonations parameters was performed. A new model for ignition delay time based on multivariate regression was implemented and validated. ddtFoam library and OpenFoam software were used to conduct 2D and 3D simulations. Velocities obtained from the experimental results were close to CJ predictions. The analysis of simulations results showed that the new detonation model gave results in good agreement with the experiments. Identical velocities were obtained in 3D and 2D simulations of 30% hydrogen in air, while for 66% of hydrogen in oxygen the 3D simulation gave velocity larger by about 100 m/s than the 2D case. This was caused by coarser grid in 3D simulation.

6.0 ACKNOWLEDGMENTS

Funding for this investigation was provided by National Centre for Research and Development agreement in project number. DOBR-BIO4/052/13073/2013 dated 23.12.2013 r.: "Innovative security technologies before the explosion, including sensitive objects", performed in Scientific and Research Center for Fire Protection - National Research Institute in Józefów/Poland.

7.0 REFERENCES

1. Tete A. D., Deshmukh A. Y., Yerpude R. R., Design and Implementation of Sensor for Velocity of Detonation Measurement, IOSR Journal of Electrical and Electronics Engineering, 2014
2. Clavin P., Theory of Gaseous Detonations, Université d'Aix-Marseille, 2004
3. Fickett W., Davis W., Detonation: Theory and Experiment, University of California Press, Berkeley, California, 1979
4. Shepherd J. E., Chemical Kinetics of Hydrogen-Air-Diluent Detonations, Progress in Astronautics and Aeronautics, American Institute of Aeronautics and Astronautics, 1986
5. OpenFoam. The Open Source CFD Toolbox. User Guide, Version 2.1.1, 2012
6. Wilcox D. C., Turbulence Modelling for CFD, DCW Industries, La Cañada Flintridge, 2006
7. Ettner F., Vollmer K. G., Sattelmayer T., Numerical Simulation of the Deflagration-to-Detonation Transition in Inhomogeneous Mixtures, Technische Universität München, Garching, 2014
8. Toro E. F., Spruce M., Speares W., Restoration of the contact surface in the HLL-Riemann solver, Cranfield Institute of Technology, Cranfield, 1993
9. Weller H. G., Tabor G., Gosman A. D. and Fureby C., Application of a Flame-wrinking LES Combustion Model to a Turbulent Mixing Layer, Symposium on Combustion, 1998
10. Uyanik, G.K. and Neşe G., A study on multiple linear regression analysis, 4th International Conference on New Horizons in Education, 2013
11. Ostertagová E., Modelling using Polynomial Regression, Modelling of Mechanical and Mechatronics Systems, 2012
12. http://www.cantera.org/docs/sphinx/html/index.html, web page, accessed 21.03.2017
13. http://shepherd.caltech.edu/EDL/public/cantera/mechs/cti/web/h2air_highT.cti, web page, accessed 21.03.2017
14. http://shepherd.caltech.edu/EDL/public/cantera/mechs/cti/web/h2o2_highT.cti, web page, accessed 21.03.2017
15. Smith G.P, Golden D.M. et al., http://www.me.berkeley.edu/gri_mech/, web page, accessed 21.03.2017
16. Slack, M. and Grillo, A., Grumman Research Department Report RE-537, Investigation of Hydrogen-Air Ignition Sensitized by Nitric Oxide and by Nitrogen Dioxide, 1977
17. Asaba, T., Gardiner, W.C. Jr., and Stubbeman, R.F., 10th Symposium (International) on Combustion, p. 295, 1965
18. http://shepherd.caltech.edu/EDL/public/cantera/html/SD_Toolbox/, web page, accessed 21.03.2017