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Original Article

Detonation cell size model based on deep neural network for hydrogen, methane and propane mixtures with air and oxygen

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ABSTRACT

The aim of the present study was to develop model for detonation cell sizes prediction based on a deep artificial neural network of hydrogen, methane and propane mixtures with air and oxygen. The discussion about the currently available algorithms compared existing solutions and resulted in a conclusion that there is a need for a new model, free from uncertainty of the effective activation energy and the reaction length definitions. The model offers a better and more feasible alternative to the existing ones. Resulting predictions were validated against experimental data obtained during the investigation of detonation parameters, as well as with data collected from the literature. Additionally, separate models for individual mixtures were created and compared with the main model. The comparison showed no drawbacks caused by fitting one model to many mixtures. Moreover, it was demonstrated that the model may be easily extended by including more independent variables. As an example, dependency on pressure was examined. The preparation of experimental data for deep neural network training was described in detail to allow reproducing the results obtained and extending the model to different mixtures and initial conditions. The source code of ready to use models is also provided.

1. Introduction and motivation

One of the dangers connected with nuclear power plants is hydrogen detonation that threatens the integrity of the containment building. A loss-of-coolant accident can cause hydrogen generation in a reaction between steam and the fuel-cladding inside the reactor pressure vessel [1]. The concentration of hydrogen can then reach the detonation limits and pose a large threat.

Numerical investigations of combustion are very important in risk assessment and loss prevention. Simulations and computer modeling allow us to consider many scenarios under different conditions with much lower costs and less time. CFD models for large scale geometries were developed and proven to give results in good agreement with experimental data. Venetsanos et al. [2] proposed source, dispersion and combustion modeling techniques regarding hydrogen explosions and validated their results against a real explosion which occurred in 1983 in Stockholm, Sweden. Molkov et al. [3] developed a model of vented gaseous deflagrations with inertial vent covers which are a very frequent scenario in process safety and risk assessment. Another validation of a CFD model of gas dispersion and explosion was performed by Middha et al. [4], who ran blind simulations and carried out experiments to check the accuracy of the model. The results obtained in his investigation showed that the model could accurately predict pressure profiles. Large scale CFD modeling of detonation was performed by Żbikowski et al. [5] In his work, a 3D detonation LES-based model was developed and verified against experimental data, showing good agreement and proving that large scale 3D simulations can be used in risk assessment regarding detonation. It implies that modeling and numerical computations in general are a very useful and needed tool in investigating detonation.

Detonation is one of the most dangerous types of combustion. In this phenomenon, a supersonic wave compresses and heats up flammable gas causing autoignition. Intense combustion, which continuously supports the shock [6], occurs because the chemical reaction rate is exponentially dependent on temperature [7]. The autoignited mixture then forms a reaction front, which follows immediately after the shock wave. Typical detonation parameters involve very high pressure and velocity of the order of 20 bar and 2000 m/s, respectively. Actual values depend on mixture composition and initial conditions.

The detonation wave is an unstable and three dimensional

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structure, where Mach stems, transverse waves and incident shocks collide with each other, forming triple points and creating detonation cells. The size of these cells depends on fuel and oxidizer properties, as well as on mixture concentration. The detonation cell size λ is the most often used criterion in assessing the ease with which a mixture can be detonated, called detonation sensitivity or detonability. A number of empirical formulas have been developed in order to correlate the detonation cell size with the possibility of the initiation of detonation in a given geometry [8,9].

Taking the above into consideration, many studies have attempted to develop empirical models based on experimental measurements, capable of calculating detonation cell sizes with satisfactory accuracy. Shchelkin and Troshin [10] were the first to propose that the detonation cell sizes can be correlated with the reaction zone length calculated using the Zeldovich-von Neuman-Döring (ZND) model [11]. Shepherd [6] considered it in a greater detail, discussing multiple definitions of reaction length. His work also included calculations based on these assumptions for various fuels. It can be concluded that the choice of the constant A, which relates the reaction length with the detonation cell size, is crucial and challenging. This coefficient varies with different fuels, oxidizers and concentrations, which makes it useful only for a narrow fragment of specific conditions. Gavrikov et al. [12] introduced a generalization of this model. It was proposed that the constant A could be made a function of two stability parameters: dimensionless effective activation energy and a parameter describing the relation between chemical energy and initial thermal energy of the combustible mixture. This approach resulted in a model which gave satisfactory results for a wide range of mixtures and concentrations. However, the question of the right reaction length definition is still open. Moreover, his model introduced new uncertainty: selection of detonation velocities which are needed to calculate effective activation energy. Although Gavrikov et al. chose values which gave the best correlation between experimental cell widths and reaction lengths, the problem of selecting these velocities still persists. For example Yu et al. [13] chose in their work different values than Gavrikov. All models mentioned so far are likewise dependent on the detailed chemical reaction mechanism selection and its error, which is seldom taken into consideration during such analyses but can be significant. Comparison of different chemical mechanisms, their relationships with initial conditions, equivalence ratio etc. is presented for example in the work of Olm et al. [14] and in recent publications of Jach et al. [15] and Rudy et al. [16]. It is apparent that all models which are dependent on chemical mechanisms introduce errors that stem directly from the use of this method. In addition, the method proposed by Gavrikov requires the multiplication of the reaction length and the coefficient dependent on the effective activation energy in order to obtain detonation cell sizes. This not only introduces two kinds of errors for each factor (uncertainty of reaction length/detonation velocity selection and the error from chemical mechanism), but also these errors are then multiplied. Another disadvantage of models that require calculation of the effective activation energy or the reaction length is that these calculations are often time consuming. It concerns the computation time, which can be significant, especially for detailed mechanisms with many reactions as well as developing scripts for calculation of these parameters. There are no standard approaches to these problems, so minor differences in implementations can result in a different values for these properties. Consequently, it produces different values of detonation cell sizes, which leads to non-repeatable studies. In their recent work, Yu et al. [13] proposed a model based on Support Vector Machines, which showed better performance in comparison with their experimental data than model made by Gavrikov et al. Unfortunately, their model still requires calculation of the effective activation energy. There is a need to develop a more robust model.

Recent progress in machine learning showed many applications in a wide variety of areas, where the results obtained by neural networks are more accurate and revolutionary. These solutions also found their use in engineering, where they either make modeling easier and faster or allow to model what previously was considered impossible. As an example, a special type of neural networks called Convolutional Networks [17] was used in CFD code based on the Euler equations developed by Tompson et al. [18]. Those networks were first trained using data from standard 3D simulations, and then used to predict the pressure field in the resulting CFD model. This method made the simulations orders of magnitude faster, the results obtained were in good agreement with original data and the model performed well in other cases as well. The next example of CFD code enhanced with machine learning is a work by Shang et al. [19], who found that such combination can be used in two-phase flows of water and vapor. They trained two artificial neural networks during the process of solving boundary and conservation equations and, as a result, could predict enthalpy and pressure in any position inside the domain with good accuracy. Another example is a study by Elkamel et al. [20], where an artificial neural network model was developed in order to simulate the process of hydrocracking unit in an oil refinery. Their model could successfully predict properties and yields of products of such processes (e.g. iC, nC, Diesel, light and heavy naphtha etc.) which are crucial in process optimization, catalyst selection, planning and control, with the maximum average percent error of 8.71%. Another industrial application of neural networks was described by Ibargüengoytia et al. [21]. In their work, a virtual sensor was developed to measure and report the current value of viscosity in a fossil fuel power plant. A virtual sensor is in fact a computer program which takes inputs from real sensors and outputs a value of interest. It is especially useful for properties which are hard or impossible to physically measure in real time. They used historical laboratory data to train their Bayesian network and obtained a very good estimator, which was later installed in the Tuxpan Power Plant in Veracruz, Mexico. A successful application of a genetic algorithm (GA) in the combustion modeling was presented by Elliott et al. [22]. In their research, GA was used in optimization of new kinetic reaction mechanisms, whereas measured ignition delay times served as a basis for the optimization process. The result of their work was an algorithm that could output reaction rate coefficients for the combustion process in order to make the chemical mechanism most accurate for calculating ignition delay times and species concentration.

The main objective of this study was to propose a new detonation cell size model, based on a deep neural network, for hydrogen, methane and propane mixtures with air and oxygen. It allows for more accurate and much faster calculations than standard approaches based on detailed chemical mechanisms and could also be extended to any other mixture and conditions, which we prove in this work.

2. Experimental data sources

Experimental data for hydrogen-air, methane-oxygen and propane-oxygen was obtained during experiments conducted in a 9 m long detonation tube with 0.17 m of inner diameter [23]. 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 took 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. 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 approximately 25°C.

Detonation cell sizes for propane-air and methane-air mixtures were obtained from literature. Knystautas et al. [24] measured detonation cell size and predicted critical tube diameters, critical initiation energy and detonability limits of hydrocarbon-air mixtures, and their results of propane-air mixture measurements were used in this work. The cell sizes of methane-air detonation were taken from the work of Zipf et al. [25], who performed extensive experiments of at NIOSH Lake Lynn Laboratory and determined detonation velocity, pressure, cell sizes and detonability limits of that mixture.

Additional data for the extended model, where the dependency on initial pressure was introduced, was gathered from literature. Measurements of detonation cell sizes for methane-oxygen mixtures at pressure lower than atmospheric were obtained from the work by Wang et al. [26]. For hydrogen-air mixture, data found in the article by Stamps and Tieszen [27] was used.

3. Preparation of data and feature engineering

Every machine learning model performance is highly dependent on the number of examples and quality of the data on which it is trained. A small number of training examples results in a model which cannot generalize well when it encounters new data to make predictions. An artificial neural network is an extremely flexible algorithm. As proven in the Universal Approximation Theorem [28], it is capable of approximating continuous functions on the Euclidean space. Being very powerful, such algorithm requires even more data than simpler machine learning models like, for example, logistic regression, Support Vector Machines (SVM) or Random Forest. Taking these properties of neural networks into consideration, special emphasis was put on the preparation of data in this work. The steps taken in order to obtain a satisfactory dataset to train the model are listed and described below:

- approximation of experimental data
- approximation of the standard deviation of experimental data
- data simulation
- generating more features using Cantera [29].
- merging data from all mixtures into one dataset
- choosing significant features for detonation cell prediction

During experimental investigations of detonation cell sizes, the number of collected measurements is usually lower than 100. This number of observations is definitely too small to be used as training data for a neural network. Data simulation needed to be performed in order to increase the number of samples. The first step in our approach was to approximate the experimental data. This approximation involved determining a polynomial of the order equal to the number of experimental points - 1 for a given mixture. Then, this polynomial approximation was also performed for the standard deviation (SD). For propane-air and methane-air data obtained from literature, we assumed that the SD can be estimated as in the widely used formula (1), known as the range rule of thumb [30].

$$SD \approx \frac{max - min}{4} \tag{1}$$

As a result, the polynomial approximations obtained could be used to perform data simulation. The simulation step assumed that, for every given concentration, cell sizes followed the Normal Distribution, whose probability density function (PDF) is described with formula (2):

$$f\left(x\middle|\mu,\sigma^2\right) = \frac{1}{\sigma\sqrt{2\pi}} e^{-(x-\mu)^2/2\sigma^2} \tag{2}$$

where μ (mean) and σ (standard deviation) were calculated using the polynomial approximation of detonation cell sizes and their standard deviations, accordingly. A total of 1000 points per mixture was generated using this approach, with random sampling from an individual PDF for every distinct value of fuel concentration. An exemplary illustration of the generated data is shown in Fig. 1.

One of the means to improve predictive power of a machine learning algorithm is feature engineering. It is a term which encapsulates all actions of refining, transforming, adding and removing the independent variables in order to make them more useful for the algorithm. In the present study, Cantera and SDToolbox [31] software was used to generate more input features for a given mixture and fuel concentration. These inputs provided more information for the model, particularly information related to mixture properties depending on the fuel - oxidizer ratio. Generated inputs were as follows: adiabatic flame temperature, Chapman-Jouguet (CJ) velocity, CJ temperature and CJ pressure, all as a function of the fuel concentration. Despite the fact that these values are also affected by the error related to the chemical mechanisms calculations, they are not influenced by any uncertainty related to the assumptions (eg. velocities in Ea/RT or reaction length definition). Also, these are basic, theoretical mixture properties where error does not accumulate during further multiplication and other operations. The next step was to merge data for all mixtures into one dataset. In order to differentiate between mixtures, new input variables were introduced: h2air, ch4air, ch4o2, c3h8air and c3h8o2, with a one-hot encoding (1 for chosen mixture, 0 for any other). The last step was to choose the best features as the final inputs to the model. The numerical and visual analysis of correlations between inputs and outputs showed that adiabatic flame temperature gave the most substantial contributions to the accuracy of the predictions. This was due to the fact that all other variables were closely, and nearly linearly, correlated to the fuel concentration so that they would not add any significant information to the inputs. Also, attempts were made to include effective activation energy in order to assess its influence on the end results, but including this term did not noticeably improve model performance on the test set. In the end, only the adiabatic flame temperature was kept as an additional input variable. The rightness of this choice was further confirmed during model evaluation.

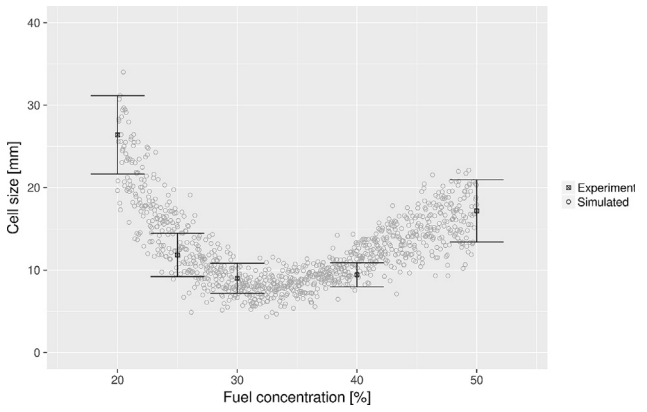

Fig. 1. Simulated 1000 cell sizes for $H_2 - air$, as a function of fuel concentration.

4. Model construction, tuning and training

The basic assumptions for the model were as follows:

- initial conditions: 1 atm, 300 K
- the number of inputs equal to 7 (adiabatic flame temperature [K], volumetric fraction of fuel and 5 kinds of mixtures: propane-air, propane-oxygen, methane-air, methane-oxygen and hydrogen-air
- one output - $log_{10}(detonation\ cell\ size\ [mm])$
- activation functions for all hidden layers: hyperbolic tangent
- identity function for the output layer

As detonation cell sizes for the examined mixtures varied from 1 to 1000 mm, as presented in Table 1, it was decided that the output of the model would be log_{10} in order to enable the model to converge faster and obtain better results. The detailed structure of the model (the number of hidden layers, the number of nodes in each layer and the L2 regularization parameter [32]) was determined using a hyperparameter grid search [33]. The constraints imposed on these parameters were:

- the number of hidden layers between 1 and 4
- the number of nodes (equal in every hidden layer) between 3 and 14
- the regularization parameter: 1e-3, 1e-4, 1e-5, 1e-6, 1e-7 or 0

FCNN4R package [34] was used for model development and calculations. Every combination of the above hyperparameters was evaluated on the training set with the use of a 5-fold cross validation [35], which is a widely known technique of measuring the performance of algorithms on different subsets of training data in order to avoid overfitting. Overfitting is observed when models perform very well on the data used to train but fail to generalize well on the data they have not seen before. The whole dataset of 5000 examples was divided into train and test sets in a proportion of 80/20. The data was shuffled randomly before the split and divided in such a way that the test set contained the same number of samples from each mixture. The chosen optimization algorithm was Rprop [36], which was used to minimize the mean squared error (MSE) between predicted and true cell sizes. Prior to model tuning and training, the data was scaled to a range [-1,1] in order to decrease calculation time of the training. After tuning, the optimal hyperparameters were as follows: 2 hidden layers, 7 nodes in each of them and 1e-6 L2 regularization coefficient. Further manual tuning allowed for reducing the number of neurons for the second hidden layer to 3 nodes, without a noticeable loss of accuracy. The schema of the final model is presented in Fig. 2. The structure of the model can be interpreted as follows: the first hidden layer handles the same number of features as the input layer (7->7), the second hidden layer compresses all mixture type features into one while retaining the rest (7->3). This is our proposed methodology for extending this model as we show in section 6.

In addition to the main model, which takes all fuels into account, models for specific mixtures were developed in order to compare their effectiveness and accuracy. Every one of the individual models underwent the same process of hyperparameters tuning as the main model.

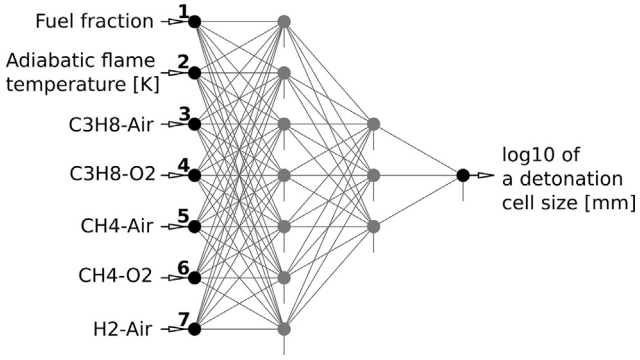

Fig. 2. Final model schema.

5. Model validation

After tuning and choosing the optimal hyperparameters, all models were evaluated on the same test dataset, which contained the same number of observations for each mixture. Statistics presenting models performance are shown in Table 2. R-squared (R^2) metric indicates how well the model fits the data. It can be seen that the main model and individual models were capable of producing good representation of detonation cell sizes. R^2 for 3 mixtures: methane-air, propane-air and propane-oxygen amounts to above 95%, which indicates a very good fit to the data. For methane-oxygen it is around 88% for both models. Hydrogen-air mixture achieved a lower value for the metric: 79%, which was caused by a large standard deviation of measurements for this mixture (as seen in Fig. 1). As a result, the hydrogen-air mixture produced the largest mean absolute percentage error (MAPE): 14.3%. For all other mixtures, this error is below 9%. Comparing individual models metrics with the performance of the main one, it can be seen that the construction of a universal model for all mixtures did not introduce additional errors. For all mixtures, performance of both models was approximately the same, with minor differences in mean absolute error (MAE) and R-squared.

Comparisons of all models performance, including calculations based on Gavrikov's model, are presented in Figs. 3–7 and in Table 3. Experimental measurements were shown with their corresponding standard deviations. The analysis of these figures confirmed that the main model and models for specific mixtures have the same performance. It can likewise be seen that their predictions agree with the experimental data. In most cases, calculated detonation cell sizes fell within bounds of the experimental standard deviations. These errors were larger only for propane-air and methane-air on Figs. 3 and 5, respectively. The comparison of the experimental values with the Gavrikov's model showed that its performance was noticeably worse. For methane-air (Fig. 5) and hydrogen-air (Fig. 7) mixtures, detonation cell

Table 1
Ranges of detonation cell sizes and standard deviations of analyzed mixtures.

Mixture	Min. cell size [mm]	Max. cell size [mm]	Min. SD [mm]	Max. SD [mm]
H_2 - air	9	26.4	1.5	4.7
CH_4 - air	209.2	999.3	9.5	67.3
CH_4–O_2	2.9	8.3	0.3	0.9
C_3H_8 - air	52.9	440.7	2.6	22
C_3H_8–O_2	1.1	3.5	0.1	0.3

Table 2
Models performance metrics on the test dataset.

Mean absolute error [mm]					
	H_2 - air	CH_4 - air	CH_4–O_2	C_3H_8 - air	C_3H_8–O_2
Main model	1.68	25.53	0.41	5.31	0.099
Individual model	1.57	26.34	0.36	5.33	0.1
Mean absolute percentage error [%]					
Main model	14.3	5	9.8	4	8.2
Individual model	14.3	5	9.7	4	8.1
R-squared					
Main model	0.79	0.97	0.88	0.99	0.96
Individual model	0.78	0.96	0.89	0.99	0.95

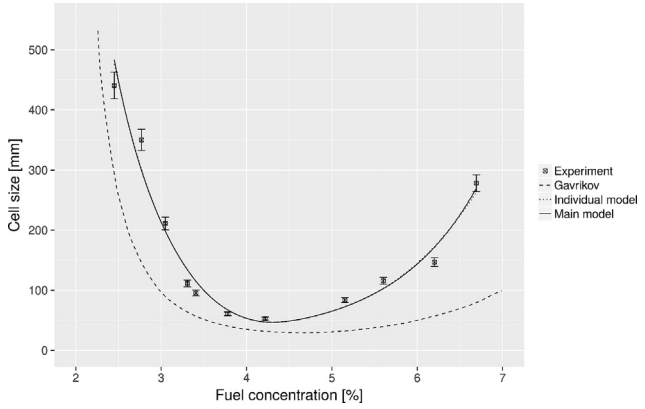

Fig. 3. Detonation cell sizes comparison for C_3H_8-air mixture, Gavrikov's model from Ref. [24].

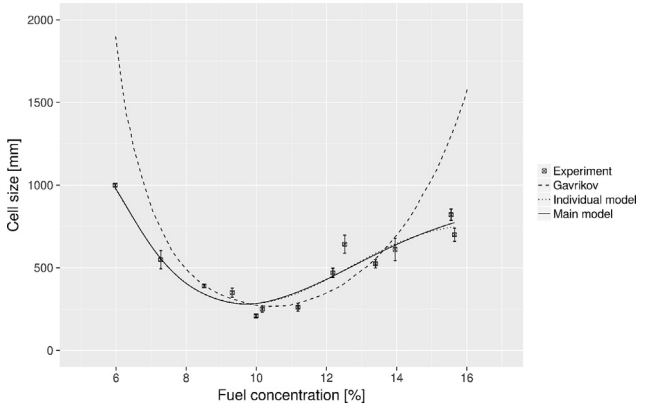

Fig. 5. Detonation cell sizes comparison for CH_4-air mixture, Gavrikov's model from Ref. [25].

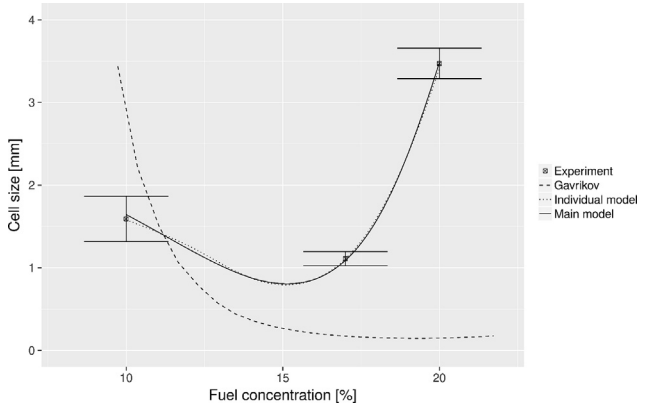

Fig. 4. Detonation cell sizes comparison for C_3H_8–O_2 mixture, Gavrikov's model from Ref. [13].

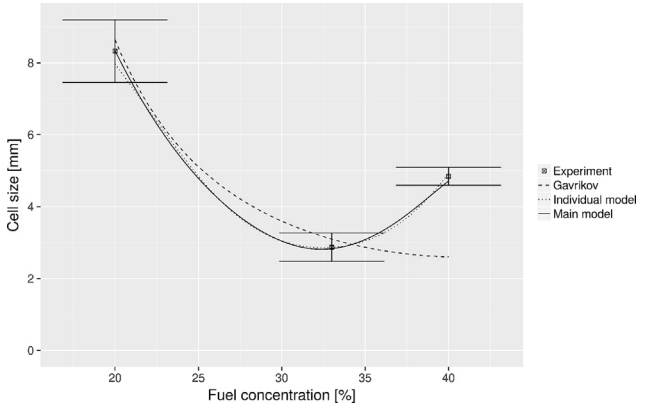

Fig. 6. Detonation cell sizes comparison for CH_4–O_2 mixture, Gavrikov's model calculated. Mechanism used: GRI-MECH 3.0 [37].

sizes calculated using the Gavrikov's method followed the overall trend, and could be considered acceptable. As can be seen in Fig. 6, the cell size for the rich methane-oxygen mixture was approximately 2 times smaller than the experimental value. For the remaining propane-air (Fig. 3) and propane-oxygen (Fig. 4) mixtures, the relative error of Gavrikov's model in comparison with the experiments was larger than 50%.

More detailed, statistical comparison of all models as well as the mean standard deviations from experiments are presented in Table 3. It confirms the conducted analysis and presents quantitative results. It can be noticed that the MAPE of Gavrikov's models is 3–14 times larger, and for propane-oxygen it is even 50 times larger than the MAPE of the models developed in this study. The largest MAPE generated by the neural net model was for methane-air and propane-air, 13.9% and 12.3%, respectively. This is due to more irregular detonation cell sizes distribution along fuel concentration for these mixtures.

6. Model extension

In order to check the extensibility of the model, pressure dependency was chosen as an additional feature. A small amount of the available data in the literature described at the end of section 2 allowed for considering only two mixtures in this case: methane-oxygen and hydrogen-air. When choosing the model structure, the number of hidden layers and nodes was determined without the use of model tuning, but following the methodology pointed out in section 4. Based on that methodology, it was concluded that

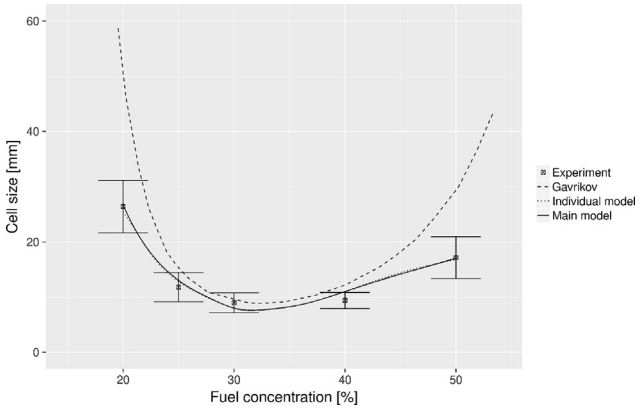

Fig. 7. Detonation cell sizes comparison for H_2-air mixture, Gavrikov's model from Ref. [12].

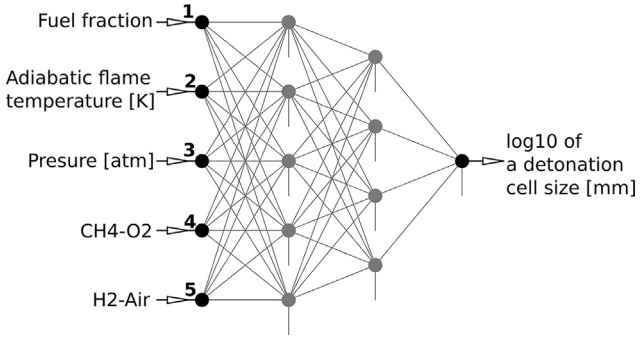

Fig. 8. Extended model schema.

the number of hidden nodes in the first hidden layer should be 5 (the same as the number of inputs) and in the second hidden layer it should be 4 (mixture inputs compressed into one node). The final structure is shown in Fig. 8.

As can be seen in Table 4, the extended model showed good, consistent performance on test data. "Atmospheric pressure" row represents the case in which the model was validated against the data involving atmospheric pressure and varying fuel concentration. The experimental data in this case was the same as in the main model. We can see that MAE, MAPE and R2 for hydrogen-air differed by respectively 0.16, 0.3 and 0.01. These differences are not significant and result from random train/test data split and from the discrepancies in the model structure. For methane-oxygen mixture, MAE and MAPE differ by 0.01 and 0.1 while R2 is higher by 0.01. These results show that including additional dependent variable in our model did not cause any diminishing of the previous performance. The same conclusions can be drawn from results in Table 5 and in Figs. 9 and 10, which show model performance in comparison with experiments. There are no significant differences between the extended and the main model based on those metrics. The "varying pressure" case concerned the dependency on pressure, while keeping the fuel concentration constant. The values in tables for this case were averaged for all examined concentrations. In Table 4 it can be seen that MAEs were larger than for the constant pressure case, but it was caused by much larger cells for lower pressures (up to 10 times). Moreover, detonation cell sizes for hydrogen-air for 17.4% concentration were about 10 times larger than for 30% as may be seen in Fig. 9. Taking these two points into consideration, MAPE is considered to be a more representative metric in this case as the values obtained were approximately half the values of the atmospheric pressure case. For hydrogen-air MAPE, was 8.3% and for methane-oxygen it was 5.2%. Once again, from Table 5 it can be concluded that the developed model is accurate. All values of MAE are lower that their corresponding standard deviations from the experimental measurements with only one exception of methane-oxygen mixture for the varying pressure validation. The MAE in this case was 1.63 mm, while the SD was 1.13 mm.

Table 4
Extended (pressure) model performance metrics on the test dataset.

Mean absolute error [mm]		
	H_2 - air	CH_4 - O_2
Atmospheric pressure	1.84	0.42
Varying pressure	6.65	0.96
Mean absolute percentage error [%]		
Atmospheric pressure	14.6	9.9
Varying pressure	8.3	5.2
R-squared		
Atmospheric pressure	0.78	0.89
Varying pressure	0.91	0.99

Table 5
Extended (pressure) model performance metrics on experimental data.

Mean absolute error [mm]		
	H_2 - air	CH_4–O_2
Atmospheric pressure	1.11	0.44
Varying pressure	3.06	1.63
Mean absolute percentage error [%]		
Atmospheric pressure	7.9	6.9
Varying pressure	5.9	5.7
Mean standard deviations of experimental measurements [mm]		
Atmospheric pressure	2.88	0.5
Varying pressure	9.1	1.13

Table 3
Models performance metrics on experimental data.

Mean absolute error [mm]					
	H_2 - air	CH_4 - air	CH_4 - O_2	C_3H_8 - air	C_3H_8 - O_2
Main model	0.85	55.87	0.06	19.73	0.028
Individual model	0.98	56.14	0.14	19.51	0.022
Gavrikov	8.65	214.68	0.93	92.41	1.86
Mean absolute percentage error [%]					
Main model	8	13.9	1.4	12.3	1.8
Individual model	8.4	13.7	2	12.4	0.8
Gavrikov	45.8	31.4	19.2	51.5	87.8
Mean standard deviations of experimental measurements [mm]					
	2.88	31.12	0.5	8.85	0.18

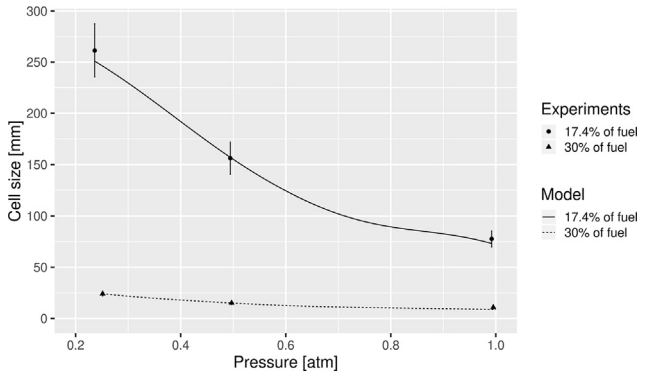

Fig. 9. Detonation cell sizes comparison for the extended model, H_2-air mixture.

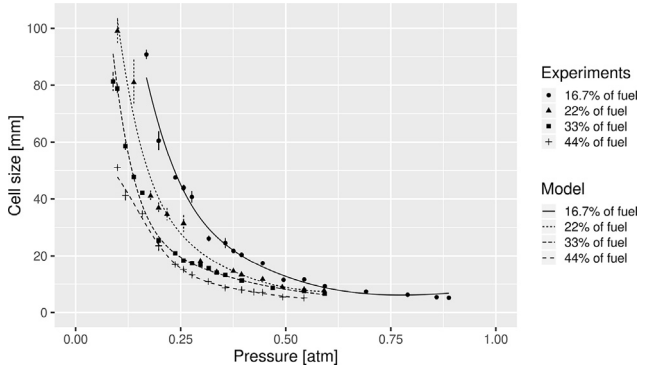

Fig. 10. Detonation cell sizes comparison for the extended model, CH_4–O_2 mixture.

7. Conclusions

In this work, a new detonation cell size model for hydrogen, methane and propane mixtures was developed and validated. The model is based on an deep neural network and requires fuel fraction, adiabatic flame temperature [K] and mixture type (i.e. an indication whether it is hydrogen-air, propane-oxygen etc.) as input parameters for initial conditions 1 atm and 300 K. Moreover, an extension of this model was also developed in order to check its flexibility and availability to include pressure as an additional dependent variable. The results proved that presented models were capable to predict detonation cell sizes for all mixtures concerned with the smallest error. In addition to better accuracy, the advantages of this approach are that the models are efficient and do not require any calculation of the effective activation energy or the reaction length. It implies that these models are not influenced by errors and uncertainties of different definitions of these properties, and are also free from errors introduced by chemical mechanisms. The only property that needs to be calculated is the adiabatic flame temperature. These models can also be easily updated when new experimental results are available, or extended to more mixtures/different initial conditions as was proved in this work. The only requirement is a large amount of experimental measurements. Then, following the methodology described in detail in this study, it is possible to properly preprocess these measurements and perform training of a new model or update the weights of the existing one.

Acknowledgments

Calculations were carried out at the Academic Computer Centre in Gdańsk.

Appendix

The two models developed in this study (the main model and the extended model) are available on github as C source code under the following address: https://github.com/konradmalik/ann-detonation-cell-sizes.git.

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