Predicting the Detonation Cell Size of Biogas-Oxygen Mixture Using Machine Learning Models

Stanislaw Siatkowski, Krzysztof Wacko, Jan Kindracki
Institute of Heat Engineering, Faculty of Power and Aeronautical Engineering,
Warsaw University of Technology
Warsaw, Poland

1 Introduction

As countries across the globe struggle to fulfill the goal of achieving carbon neutrality by 2050 [1], biogas is considered to be a promising, alternative fuel. Biogas is a product of anaerobic digestion in the presence of bacteria [2] of biomass derived from sources like agriculture, forestry or similar source [3]. It consists mostly of CH_4 and CO_2, typically ranging 35% ÷ 70% of volume for CH_4 and 15% ÷ 50% for CO_2. With those two gases being the main ingredients, usually biogas also contains a number of different contaminants that are dependent on the biomass origin and production processes [4]. Thanks to the fact that the net balance of CO_2 released into the atmosphere during its combustion is close to zero and that as an energy source it is weather-independent and easily storable it is attracting more and more attention globally [5].

At the same time, the number of studies on biogas detonation is extremely limited. Wahid et al.[6] presented results from experiments with biogas - oxygen mixture diluted at various percentages with N_2. It was shown that the correlation between cell size and the percentage of N_2 in the mixture was positive, meaning that when the N_2 percentage increased, the cell size increased as well. Wahid and Ujir [7] also compared the same biogas to natural gas with 92.7% CH_4 and propane, showing that for the same nitrogen volume in the mixture, propane presents smaller cell size. In their paper, Elhawary et al. [8] presented the results of running an experimental PDE on a biogas-oxygen mixture with various percentage of H_2 dilution. The biogas consisted of 60% CH_4 and 40% CO_2 while the dilution of H_2 ranged from 0% to 20% and was added after creating a stoichiometric biogas-oxygen mixture. They showed that the addition of hydrogen resulted in a significant decrease of the detonation cell size. During the 28th ICDERS [9] conference the authors of this paper presented the results of the extensive experimental study of biogas-oxygen mixtures that consisted of over 200 different cases. In this experiments a range of different initial pressures, equivalence ratios and biogas compositions were tested.

Correspondence to: jan.kindracki@pw.edu.pl

Being able to estimate or predict a detonation cell size is important in two aspects. First one is a topic of safety. In case of a gas leak and a ignition a suitable conditions for transition of the flame from deflagrative to detonative regime may occur. Knowledge of the detonation cell size is crucial while performing safety analysis. On the other hand, this knowledge is also important when designing a rotating detonation combustion chamber as the height of which must larger than the detonation cell size to allow for sustaining a continuous detonation [10].

The number of studies using machine learning techniques in the combustion discipline is very limited and none of them concerns biogas combustion. In this study, we present the results of creating and comparing a number of machine learning models created to predict the detonation cell size. A big dataset of cell size measurements collected from the aforementioned experimental studies was used to train and evaluate 3 types of machine learning models: Linear Regression, Support Vector Machine and Neural Network. The objective was to investigate if a that kind of technique can be used to estimate detonation cell size with sufficient accuracy. Brief overview of this study is provided below.

2 Methodology

2.1. Dataset

The dataset used in this study consisted of over 35,000 detonation cell size measurements collected during aforementioned experimental study of biogas-oxygen mixtures. The parameters that were varied during experiments were as follows:

- initial pressure p_0 from 0.6 bar to 1.6 bar: {0.6; 0.7; 0.8; 0.9; 1.0; 1.2; 1.4; 1.6},
- equivalence ratio ϕ: {0.5; 0.75; 1.0; 1.25; 1.5},
- biogas composition with percentage of CH_4 going from 40% to 70% in 5% increments with the rest being CO_2 as a 'synthetic' (without contaminants) biogas was used.

In the cases of biogas containing 40% and 45% of methane only stoichiometric mixtures were tested due to the problems with achieving stable detonation. Number of collected measurements in every case ranged from few to few hundreds. This was because the average cell size ranged from around 5 mm up to 50 mm depending on a given case set of mixture parameters. The description of an experimental setup used in the study is outside of the scope of this document but an interested reader is referred to a previous work of the authors [11], where the test stand is described in greater details.

2.2. Machine Learning Algorithms

2.2.1. Multivariate Regression

Multivariate regression is a method that predicts a quantitative response Y on the basis of a number of independent variables – predictors. It assumes that there is approximately a linear relationship between a dependent variable Y and independent variables X. This model is defined as follows:

$$Y = X*B + E$$

where the Y is a matrix of observations (in our case a vector with cell size measurements); X is a matrix with *n* rows equal to the number of observations and *k+1* columns where *k* is the number of independent variables and the additional column consists of 1s for the regression

constant; B is the a matrix of regression coefficient, on for each independent variable and E is an error matrix [12].

2.2.2. Support Vector Regression

Support Vector Machine (SVM) is a method of fitting an optimal hyperplane to the data. Input vectors X are mapped into the high-dimensional feature space Z through nonlinear mapping, chosen a priori. In case of classification the hyperplane is used to optimally separate the data points from different classes. While in case of regression the hyperplane is fitted in such a way as to minimize the distances between the plane and data points [13].

2.2.3. Artificial Neural Network

An artificial neural network consists of three types of layers: input, output and hidden layers. Nodes in input layer are passive which means that hey do not perform any operations except for passing the values fed to them further into the hidden layers. Output layer is used to read the prediction values. Number of nodes in the output layer depends on the problem, in case of this study it is one as only one value is being predicted – detonation cell size. Depending on the configuration of the nodes and connections between them in the hidden layers, different kind of ANNs can be distinguished. A network architecture used in the presented study was a Multi-Layer Perceptron (MLP). In this architecture every node in hidden layer takes feeds its outputs to all nodes in the next layer, there is no skipping layer and no feeding the output backwards. Additionally, the hidden layers do not take inputs from outside of the network. The connections between nodes contain weights by which output coming from one node to another through this connection is multiplied. Those weights show the influence of a given mode on the output value. In a node all the inputs (each being an output from previous node multiplied by a connection weight) are summed and passed to the node's activation function. Figure 1 presents a schematic of a multi-layer perceptron architecture of a neural network.

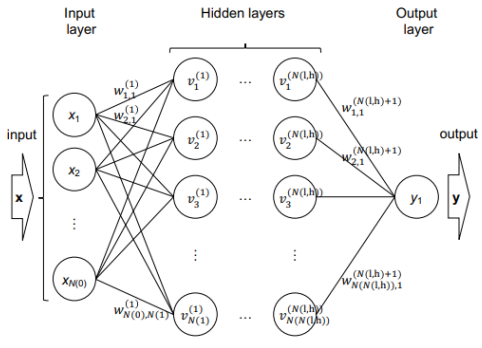

Figure 1: A schematic of a Multi-layer Perceptron type of Neural Network [14].

The process of training a neural network takes place in a number of iteration. Each iteration is divided into two steps: forward and backward propagation. In the forward propagation the network predicts output values for the training data provided for it. The next step is the backward propagation in which the aforementioned weights assigned to connections between nodes are adjusted. This is done using a cost function and aims to minimize the prediction error, that is the difference between predicted value and the actual value provided in

the training set. The training is stopped after a pre-set number of iterations or when subsequent iterations do not decrease the error anymore. Finally when the model is ready to be used, only forward pass is used to obtain the predictions.

2.3. Explanatory Variables

In the presented study two sets of explanatory variables were used on which the models were trained. First one, used directly the parameters that were being varied during experiments, that is: % o CH_4 in a biogas, initial pressure, equivalence ratio. Additionally interactions between those parameters were also included as well as some transformations of p_0 and ϕ. Finally the first set of independent variables used in models training was as follows:

$$X^1 = (\%CH_4, \phi, \phi^2, p_0, 1/p_0, ln(p_0), \phi*p_0, \phi*\%CH_4, p_0*\%CH_4)^T$$

3 Results and discussion

3.1. Model Training and Evaluation

During the study a three machine learning algorithms, as described above, were trained and tested. Despite checking two different sets of explanatory variables additionally two different treatments considering dependent variable (cell size) were researched. The first approach used the measurements directly in as a dependent variable, meaning that the number of training data points was around 28,000 (80% of 35,000 was used in training). In the second, the model was trained using average cell sizes calculated for every case from a training set. This reduced the number of training points from around 28,000 to around 200 which was the number of unique sets of parameters: initial pressure, equivalence ratio and biogas composition ($\%CH_4$). The rationale behind the second approach was that when one tries to gather the data to train a model from literature, usually only average values are available. In case of neural network, as this kind of technique usually requires a lot of data for training, it was decided to try only the first approach.

In order to evaluate model's performance a number of metrics were calculated. Those were: coefficient of determination (R^2), mean absolute error (MAE) and mean absolute percentage error (MAPE). The coefficient of determination describes how much of the variation seen in the data is explained by the model. The closer its value is to 1 the better the model is. It is calculated using following formula.

$$R^2 = 1 - \frac{\sum_i (y_i - \hat{y})^2}{\sum_i (y_i - \bar{y})^2}$$

3.2. Model Predictive Performance

Table 1 presents the summary of the performance of the optimized models on a test set. Dataset used for testing was created by setting aside 20% of the whole data set and not using it in the training process. All models, both trained on averages and raw measurements, were tested using test set of raw cell measurements. In Table 1 values of all three metrics describing model performance are presented. For every model two values of every metrics are provided, the second value shows the metric when, so called 'experimental uncertainty' was taken into account. This was assumed to be ±20% and served to take into account the fact that the cell size for a given set of mixture parameters is not only one value but rather forms a

distribution. In this approach any actual value that fell in the range of ±20% from the predicted value was assumed to be predicted correctly. It can be seen that in both cases the results are very good ranging R^2 from 0.82 up to 0.97. It is also important to note that although Neural Network gives the best results all the models are giving very similar results.

Table 1: Results on the test set without and with taking into account experimental uncertainty

Trained on	Model Type	R^2	MAE	MAPE
Averages	Regression	0.82/0.97	2.74/0.59	0.18/0.04
	Support Vector Regression	0.85/0.95	2.52/1.77	0.17/0.23
Raw Data	Regression	0.83/0.97	2.66/0.55	0.18/0.04
	Support Vector Regression	0.86/0.92	2.40/1.69	0.16/0.18
	Neural Network	0.84/0.97	2.5/0.46	0.16/0.03

Figure 2 presents predicted values plotted against the actual one for models trained on the raw data. Diagonal black line represents the ratio of predicted/actual equal to 1, namely ideal prediction. It can be seen that, as mentioned above the models perform very similar. In some cases regression overestimates while in others it is the closest to the diagonal. Due to the lack of space the results for the second set of training parameters (molar weight, entropy etc.) is not presented here but will be during the conference.

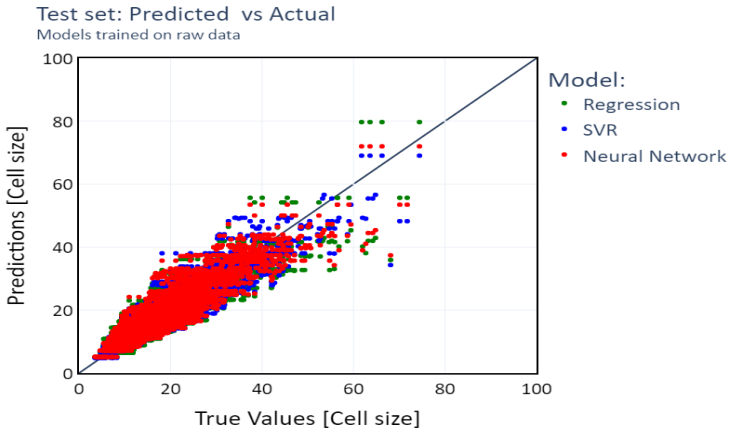

Figure 2: Results on the test set, colored by the model. Models trained on the raw data.

4 Conclusions

In this study a number of models was trained and tested. The independent variables used in the models were initial pressure, methane content, equivalence ratio and additional features based on those three. Additionally, because usually raw, experimental data is hard to obtain from literature because only averages are generally reported models trained on average values were compared to those trained on raw data. It was shown that the although the best results were achieved for Neural Network trained on raw data, models trained on averages were only marginally worse. On top of this, additional calculations of model performance were done taking into consideration the fact the cell size forms a distribution and does not takes one value. This resulted in increasing the model performance metrics even further.

References

[1] Net Zero Coalition | United Nations. https://www.un.org/en/climatechange/net-zero-coalition. Accessed Aug. 9, 2022.

[2] Gupta, K. K., Rehman, A., and Sarviya, R. M. Bio-Fuels for the Gas Turbine: A Review. *Renewable and Sustainable Energy Reviews*. 9. Volume 14, 2946–2955.

[3] Benato, A., and Macor, A. "Italian Biogas Plants: Trend, Subsidies, Cost, Biogas Composition and Engine Emissions." *mdpi.com*, 2019. https://doi.org/10.3390/en12060979.

[4] Baccioli, A., Antonelli, M., Frigo, S., Desideri, U., and Pasini, G. "Small Scale Bio-LNG Plant: Comparison of Different Biogas Upgrading Techniques." *Applied Energy*, Vol. 217, 2018, pp. 328–335. https://doi.org/10.1016/j.apenergy.2018.02.149.

[5] Norouzi, O., and Dutta, A. "The Current Status and Future Potential of Biogas Production from Canada’s Organic Fraction Municipal Solid Waste." *Energies 2022, Vol. 15, Page 475*, Vol. 15, No. 2, 2022, p. 475. https://doi.org/10.3390/EN15020475.

[6] Wahid, M. A., Ujir, H., Saqr, K. M., and Sies, M. M. Experimental Study of Confined Biogas Pulse Detonation Combustion. 2009.

[7] Wahid, M. A., and Ujir, H. "Reacting Shock Waves Characteristics for Biogas Compared to Other Gaseous Fuel." *AIP Conference Proceedings*, Vol. 1440, No. Imat 2011, 2012, pp. 90–99. https://doi.org/10.1063/1.4704206.

[8] Elhawary, S., Saat, A., Wahid, M. A., and Ghazali, A. D. "Experimental Study of Using Biogas in Pulse Detonation Engine with Hydrogen Enrichment." *International Journal of Hydrogen Energy*, Vol. 45, No. 30, 2020, pp. 15414–15424. https://doi.org/10.1016/j.ijhydene.2020.03.246.

[9] Extended Abstracts Files – 28th ICDERS. http://www.28icders.stems.cnr.it/?page_id=751. Accessed Jan. 16, 2023.

[10] Xie, Q., Wen, H., Li, W., Ji, Z., Wang, B., and Wolanski, P. "Analysis of Operating Diagram for H2/Air Rotating Detonation Combustors under Lean Fuel Condition." *Energy*, Vol. 151, 2018, pp. 408–419. https://doi.org/10.1016/j.energy.2018.03.062.

[11] Siatkowski, S., Wacko, K., and Kindracki, J. "Experimental Research on Detonation Cell Size of a Purified Biogas-Oxygen Mixture." *Energies*, Vol. 14, No. 20, 2021. https://doi.org/10.3390/en14206605.

[12] Weisberg, S. "Applied Linear Regression: Third Edition." *Applied Linear Regression: Third Edition*, 2005, pp. 1–310. https://doi.org/10.1002/0471704091.

[13] Vapnik, V. N. "The Nature of Statistical Learning Theory." *The Nature of Statistical Learning Theory*, 2000. https://doi.org/10.1007/978-1-4757-3264-1.

[14] Kawasaki, A., Hasegawa, H., Sun, H., Watanabe, H., Itouyama, N., Matsuoka, K., Kasahara, J., Matsuo, A., and Funaki, I. "Data-Driven Modeling of Reflection Point Distance Relevant to Diffracting Detonation Wave by Using Machine Learning." 2022, pp. 1–6.

[15] Goodwin, D. G., Moffat, H. K., Schoegl, I., Speth, R. L., and Weber, B. W. Cantera: An Object-Oriented Software Toolkit for Chemical Kinetics, Thermodynamics, and Transport Processes. https://www.cantera.org. Accessed Sep. 29, 2022.