

PAPER • OPEN ACCESS

# Bayesian Regularization-Trained Multi-layer Perceptron Neural Network Predictive Modelling of Phenol Degradation using ZnO/Fe<sub>2</sub>O<sub>3</sub> photocatalyst

To cite this article: Omer Al Haiqi *et al* 2020 *J. Phys.: Conf. Ser.* **1529** 052058

View the [article online](#) for updates and enhancements.

You may also like

- [Electro-Peroxone Treatment of Phenol: Process Comparison, the Effect of Operational Parameters and Degradation Mechanism](#)  
Ozge Turkey, Sibel Barç, Bahar Öztürk *et al.*
- [A comparative study on the activity of TiO<sub>2</sub> in pulsed plasma under different discharge conditions](#)  
Lijuan DUAN, , Nan JIANG *et al.*
- [Enhanced Fenton-like degradation of phenol by sulfur modified -Fe<sub>2</sub>O<sub>3</sub>/Fe<sub>3</sub>O<sub>4</sub>/R-TiO<sub>2</sub> composite coating on Ti alloy prepared by plasma electrolytic oxidation](#)  
Zhendong Wu, Jiankang Wang, Changju Chen *et al.*

Recent citations

- [Modeling the prediction of hydrogen production by cogasification of plastic and rubber wastes using machine learning algorithms](#)  
Bamidele Victor Ayodele *et al*
- [Artificial Neural Network Modeling of Thermo-catalytic Methane Decomposition for Hydrogen Production](#)  
May Ali Alsaffar *et al*
- [Radial Basis Function Neural Network Model Prediction of Thermo-catalytic Carbon Dioxide Oxidative Coupling of Methane to C2-hydrocarbon](#)  
Bamidele Victor Ayodele *et al*



The Electrochemical Society  
Advancing solid state & electrochemical science & technology

## 241st ECS Meeting

May 29 – June 2, 2022 Vancouver • BC • Canada

Abstract submission deadline: Dec 3, 2021

Connect. Engage. Champion. Empower. Accelerate.  
We move science forward



Submit your abstract



# Bayesian Regularization-Trained Multi-layer Perceptron Neural Network Predictive Modelling of Phenol Degradation using ZnO/Fe<sub>2</sub>O<sub>3</sub> photocatalyst

Omer Al Haiqi<sup>1</sup>, Abdurahman Hamid Nour<sup>1</sup>, Bamidele Victor Ayodele<sup>2</sup>, Rushdi Bargaa<sup>1</sup>,

<sup>1</sup>Faculty of Chemical and Process Engineering Technology, College of Engineering Technology, Universiti Malaysia Pahang, Lebuhraya Tun Razak, 26300 Gambang-Kuantan, Malaysia

<sup>2</sup>Institute of Energy Policy and Research, Universiti Tenaga Nasional, Jalan IKRAM-UNITEN, 4300 Kajang Malaysia

omaralhaigi@gmail.com

**Abstract.** The processing of crude oil in the onshore platform often results in the generation of produce water containing harmful organic pollutants such as phenol. If the produce water is not properly treated to get rid of the organic pollutants, human exposure when discharged could be detrimental to health. Photocatalytic degradation of the organic pollutant has been a proven, non-expensive techniques of removing these harmful organic compounds from the produce water. However, the detail experimentation is often tedious and costly. One way to investigate the non-linear relationship between the parameters for effective performance of the photodegradation is by artificial neural network modelling. This study investigates the predictive modelling of photocatalytic phenol degradation from crude oil wastewater using Bayesian regularization-trained multilayer perceptron neural network (MLPNN). The ZnO/Fe<sub>2</sub>O<sub>3</sub> photocatalyst used for the photodegradation was prepared using sol-gel method and employed for the phenol degradation study in a batch reactor under solar irradiation. Twenty-six datasets generated by Box-Behken experimental design was used for the training of the MLPNN with input variables as irradiation time, initial phenol concentration, photocatalyst dosage and the pH of the solution while the output layer consist of phenol degradation. Several MLPNN architecture was tested to obtain an optimized 4 5 1 configuration with the least mean standard error (MSE) of 1.27. The MLPNN with the 4 5 1 architecture resulted in robust prediction of phenol degradation from the wastewater with coefficient of determination (R) of 0.999.

**Keywords:** Bayesian regularization; multilayer perceptron; Artificial Neural Network; Phenol; Photocatalyst

## 1. Introduction

The upstream petroleum processing often contains mixture of chemicals that if not properly treated are very harmful to human health [1]. One of such harmful organic substance is phenol which is a very toxic substance that can cause serious health damages [2,3]. One way to remove this recalcitrant organic substance is to degrade them from wastewater under solar irradiation using photocatalysts [3,4]. This method is environmentally friendly and cost-effective compare to other chemical methods.



Content from this work may be used under the terms of the [Creative Commons Attribution 3.0 licence](https://creativecommons.org/licenses/by/3.0/). Any further distribution of this work must maintain attribution to the author(s) and the title of the work, journal citation and DOI.

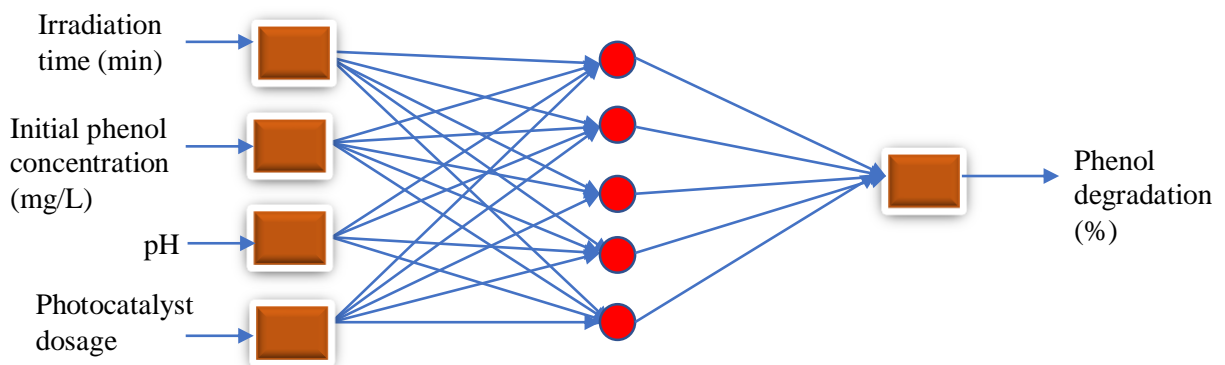
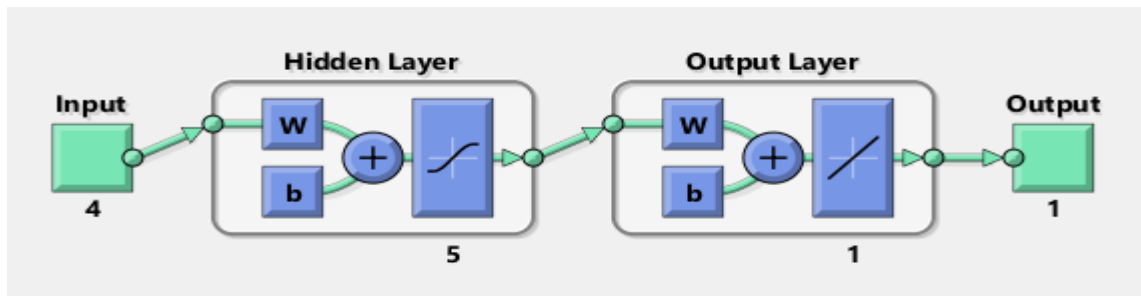
However, understanding the non-linear effect of the process parameters in the photocatalytic reaction has been a bone of contention. One way to study the effect of the process parameter on the photodegradation of the phenol for predictive modeling is using artificial neural network [5,6]. Artificial Neural Network is one of the machine learning technique that mimic the human nervous system [6]. The artificial neural network is made up of interconnectivities of hidden neurons intended to address a specific task. It has been widely applied in chemical processes [7]. Ayodele et al. [8] used artificial neural network for the prediction of CO-rich hydrogen production rate from methane dry reforming process. Schmitt et al [9]. employed artificial neural network to develop a predictive model for membrane fouling in an anoxic-aerobic membrane bioreactor treating domestic wastewater. The study revealed that the ANN model was effective in predicting the membrane fouling with  $R^2$  of 0.850. Antwi et al. [10] utilized feed forward neural network model for estimating pollutant removal in an industrial starch processing wastewater. The ANN model was found to be efficient in predicting the removal of the pollutant from the wastewater with  $R^2$  value of 0.87. To the best of the authors' knowledge, the use of ANN for predictive modeling of photocatalytic phenol degradation over ZnO/Fe<sub>2</sub>O<sub>3</sub> photocatalyst has not been reported in literature. This aim of this study is to investigate the predictive modeling of phenol degradation in an upstream wastewater using Bayesian regularization-trained multilayer artificial neural network.

## 2. Data acquisition and experimental runs

Box-Behnken experimental design was employed to generate the dataset used for the MLP predictive modeling [11]. The experimental design consists of 26 datasets comprise of the combinations of the input parameters (irradiation time, initial phenol concentration, pH, and the photocatalyst dosage) and the target (phenol degradation). Sol-gel method was employed for the synthesis of the ZnO/Fe<sub>2</sub>O<sub>3</sub> photocatalyst [12]. A 120 ml cylindrical batch reactor was used for the photodegradation experiment under solar irradiation. Stipulated dosage of the ZnO/Fe<sub>2</sub>O<sub>3</sub> photocatalyst was added to the oil field produced water and continuously stirred under dark for 60 minutes.

### 2.1 Multilayer Perceptron Neural Network Architecture

The multilayer perceptron is typical of a feed forward artificial neural network that has the capability to approximate a non-linear function [13]. The MLP architecture comprises an input layer where the signals are received, the hidden layer with capability to approximate continuous function and the outer layer. In MLP, the set of input-output pairs are often trained for the purpose of developing a learning model to determine the relationship between the inputs and the outputs [14]. During the training, the parameters of the MLP model which include the weight and bias are adjusted to minimize the predictive error. One way to measure the error is to use mean square error (MSE) [15]. The MSE measures the average of the squares of the errors between the predicted and the actual values. Algorithms such as Levenberg-Marquardt, Scale Conjugate Gradient, and Bayesian regularization can be employed for training the network [13,16]. The Bayesian regularization has the advantage of converting non-linear data by minimizing the combined errors together with the network weights in order to determine the appropriate combinations that could result be well-generalized [17]. The MLP architecture is depicted in Figure 1. It is made of the input layer (irradiation time, initial phenol concentration, pH, and the photocatalyst dosage), the hidden layer which is made of five units and the output layer (phenol degradation). Prior to the MLP configuration, the hidden layer was optimized using different numbers of neuron ranging from 1-20. The MLP architecture with the smallest hidden neuron was selected as the optimized architecture.

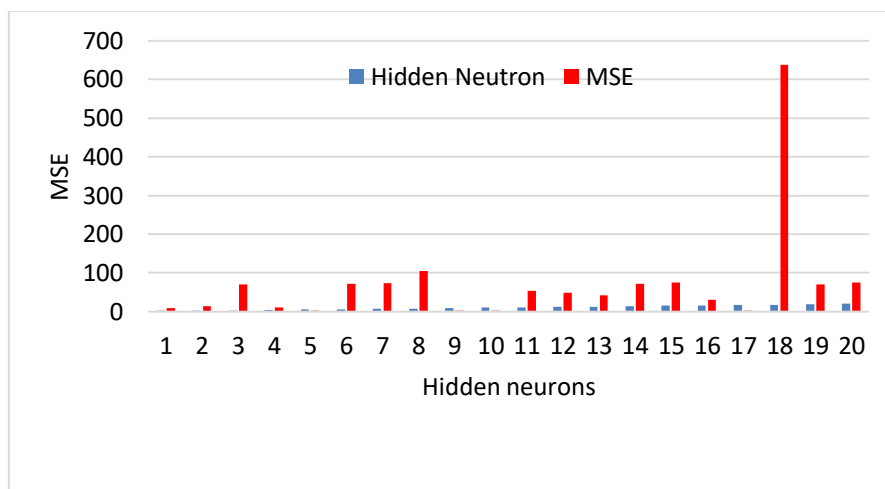


**Figure 1.** Optimized Multilayer Neural Network Architecture

### 3. Results and Discussion

#### 3.1 The network architecture

Twenty-six dataset were employed for the training of the network using Bayesian regularization algorithm. Of the 26 datasets, 70% was used for training, 15% was used for validation while the remaining 15% was used for testing. The optimization of the MLP architecture is depicted in Figure 2. Twenty different MLP model architecture were tested in order to obtain the optimized model with minimized mean standard error. The architecture with 5 hidden neurons resulted in the least MSE values of 1.27 as shown in Table 1.



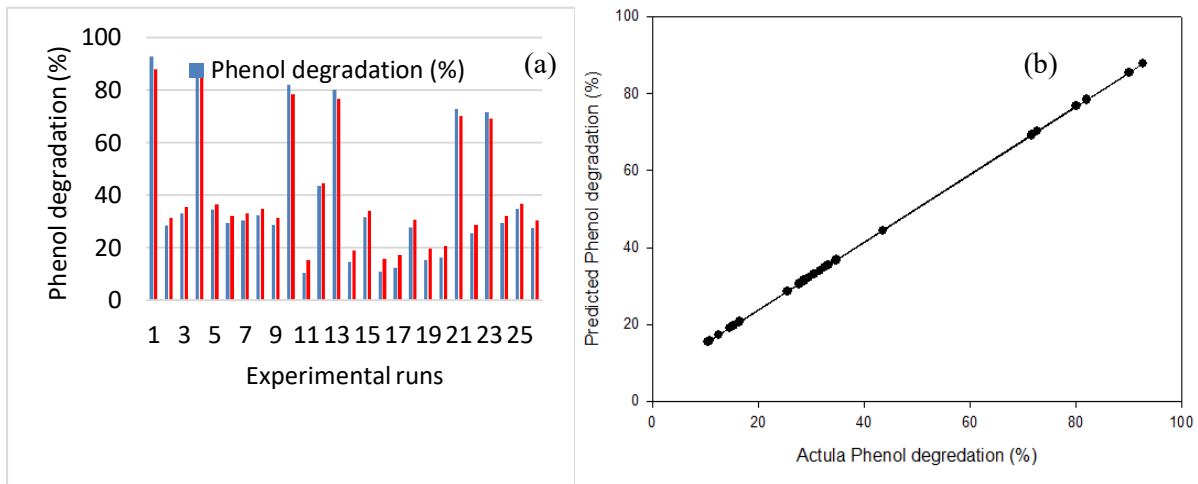
**Figure 2.** Optimization of the hidden neuron

**Table 1.** Summary of the different MLP architectures together with their MSE

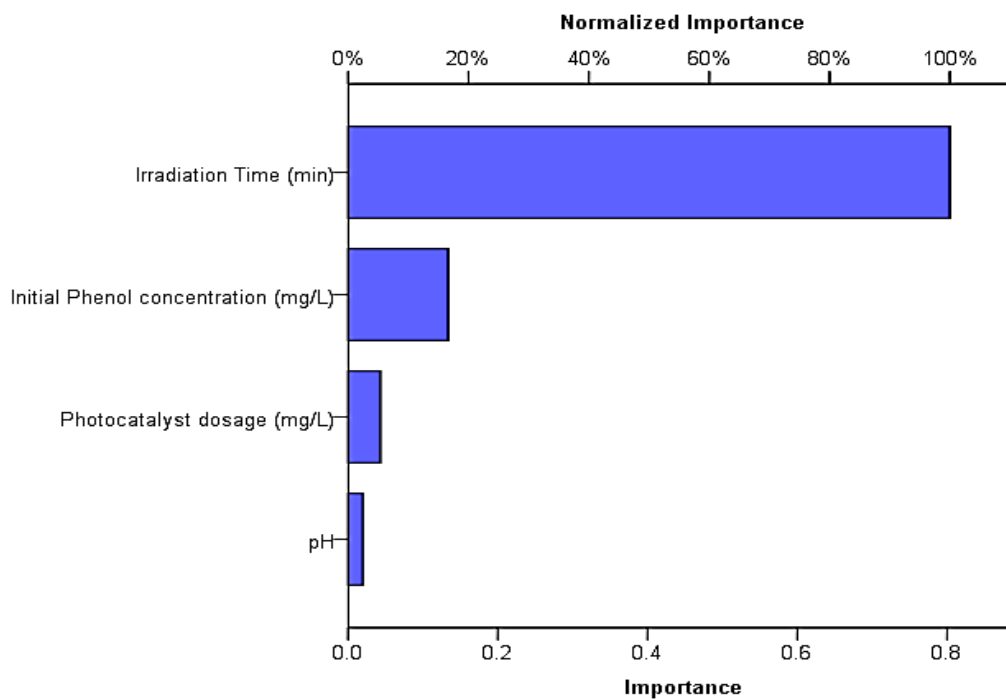
MLP Architecture	Hidden Neurons	Training		Validating		Testing	
		MSE	R	MSE	R	MSE	R
4 1 1	1	8.59	0.993	0.00	0.000	706.42	0.886
4 2 1	2	14.44	0.998	0.00	0.000	670.35	0.685
4 3 1	3	69.85	0.949	0.00	0.000	95.08	0.783
4 4 1	4	10.86	0.989	192.70	0.920	739.78	0.586
<b>4 5 1</b>	<b>5</b>	<b>1.27</b>	<b>0.999</b>	<b>19.62</b>	<b>0.983</b>	<b>19.84</b>	<b>0.999</b>
4 6 1	6	71.48	0.948	0.00	0.000	86.01	0.913
4 7 1	7	73.49	0.947	0.00	0.000	84.08	0.948
4 8 1	8	104.84	0.936	106.74	-0.982	283.38	0.974
4 9 1	9	1.31	0.999	0.00	0.000	316.65	0.945
4 10 1	10	1.45	0.998	0.00	0.000	597.98	0.725
4 11 1	11	54.41	0.947	0.00	0.000	5.03	0.998
4 12 1	12	48.10	0.963	0.00	0.000	64.00	0.992
4 13 1	13	42.24	0.968	0.00	0.000	96.47	0.794
4 14 1	14	71.61	0.928	0.00	0.000	72.60	0.958
4 15 1	15	74.87	0.945	0.00	0.000	13.39	0.916
4 16 1	16	29.86	0.979	0.00	0.000	213.90	0.625
4 17 1	17	1.53	0.998	0.00	0.000	814.32	0.448
4 18 1	18	638.09	0.941	0.00	0.000	268.85	0.945
4 19 1	19	70.36	0.946	0.00	0.000	45.48	0.889
4 20 1	20	74.76	0.941	0.00	0.000	23.43	0.982

### 3.2 MLP model performance

The MLP model performance is depicted in Figure 3 (a). It can be seen that the Bayesian regularization trained network has a robust predictive ability as shown in Figure 3. In each of the experimental runs, the predictive values of the phenol degradation are in proximity with the actual values. This is reflected in the parity plot shown in Figure 3 (b) with R values of 0.999. This implies that the predicted values are strongly correlated with the actual values. The performance of the Bayesian regularization-trained neural network can be attributed to its robustness in generalizing a non-linear function [18]. The level of importance of the input parameters based on sensitivity analysis is depicted in Figure 4. It can be seen that the irradiation time has the highest influence on the prediction of the phenol degradation. The level of importance can be ranked as irradiation time > initial phenol concentration > photocatalyst dosage > pH. The robustness of the Bayesian regularization-trained neural network has been reported for modeling explosion risk analysis of fixed offshore platform [17]. The developed Bayesian regularization-trained neural network was efficient in predicting the explosion risk analysis in the fixed offshore platform. Furthermore, Bayesian regularization trained neural network has been applied in modeling to quantify trace gas species in an oil and gas production [19]. The Bayesian regularization trained neural network was found to have a superior predictability compare to linear models.



**Figure 3.** (a) Model Performance of the MLP (b) Parity plot showing the comparing between the predicted phenol degradation and the actual values



**Figure 4.** Level of importance of the input parameters on the phenol degradation.

**4. Conclusion**

In this study the application of Bayesian regularization-trained multilayer perceptron neural network has been demonstrated. Twenty-six dataset obtained from Box-Behken design of photocatalytic degradation experiment using ZnO/Fe<sub>2</sub>O<sub>3</sub> photocatalyst was tested in the MLPNN architectures. An optimized architecture of 4 5 1 representing the input layer, hidden layer and the output layer were employed for the predictive modeling. The MLPNN model accurately predicted the phenol degradation from the wastewater. The actual phenol degradation is in proximity with the predicted values as confirmed by the R values of 0.999.

## References

- [1] Moradi V, Ahmed F, Jun MBG, Blackburn A, Herring RA. Acid-treated Fe-doped TiO<sub>2</sub> as a high performance photocatalyst used for degradation of phenol under visible light irradiation. *J Environ Sci* 2019;**83**:183–94. doi:<https://doi.org/10.1016/j.jes.2019.04.002>.
- [2] Villegas LGC, Mashhadi N, Chen M, Mukherjee D, Taylor KE, Biswas N. A Short Review of Techniques for Phenol Removal from Wastewater. *Curr Pollut Reports* 2016;**2**:157–67. doi:10.1007/s40726-016-0035-3.
- [3] Vaiano V, Matarangolo M, Murcia JJ, Rojas H, Navío JA, Hidalgo MC. Enhanced photocatalytic removal of phenol from aqueous solutions using ZnO modified with Ag. *Appl Catal B Environ* 2018;**225**:197–206. doi:10.1016/j.apcatb.2017.11.075.
- [4] Hidalgo MC, Maicu M, Navío JA, Colón G. Photocatalytic properties of surface modified platinised TiO<sub>2</sub>: Effects of particle size and structural composition. *Catal Today* 2007;**129**:43–9. doi:10.1016/j.cattod.2007.06.052.
- [5] Yilmaz I, Kaynar O. Multiple regression, ANN (RBF, MLP) and ANFIS models for prediction of swell potential of clayey soils. *Expert Syst Appl* 2011;**38**:5958–66. doi:10.1016/j.eswa.2010.11.027.
- [6] Hossain MA, Ayodele BV, Cheng CK, Khan MR. Artificial neural network modeling of hydrogen-rich syngas production from methane dry reforming over novel Ni/CaFe<sub>2</sub>O<sub>4</sub> catalysts. *Int J Hydrogen Energy* 2016;**41**. doi:10.1016/j.ijhydene.2016.04.034.
- [7] Mosavi A, Salimi M, Ardabili SF, Rabczuk T, Shamshirband S, Varkonyi-Koczy AR. State of the art of machine learning models in energy systems, a systematic review. *Energies* 2019;**12**. doi:10.3390/en12071301.
- [8] Ayodele BV, Mustapa SI, Alsaffar MA, Cheng CK. Artificial intelligence modelling approach for the prediction of CO-rich hydrogen production rate from methane dry reforming. *Catalysts* 2019;**9**. doi:10.3390/catal9090738.
- [9] Schmitt F, Banu R, Yeom I-T, Do K-U. Development of artificial neural networks to predict membrane fouling in an anoxic-aerobic membrane bioreactor treating domestic wastewater. *Biochem Eng J* 2018;**133**:47–58. doi:<https://doi.org/10.1016/j.bej.2018.02.001>.
- [10] Antwi P, Li J, Meng J, Deng K, Quashie FK, Li J, et al. Feedforward neural network model estimating pollutant removal process within mesophilic upflow anaerobic sludge blanket bioreactor treating industrial starch processing wastewater. *Bioresour Technol* 2018;**257**:102–12. doi:<https://doi.org/10.1016/j.biortech.2018.02.071>.
- [11] Ayodele B V., Cheng CK. Modelling and optimization of syngas production from methane dry reforming over ceria-supported cobalt catalyst using artificial neural networks and Box–Behnken design. *J Ind Eng Chem* 2015. doi:10.1016/j.jiec.2015.08.021.
- [12] Zhang Y, Wang D, Zhang G. Photocatalytic degradation of organic contaminants by TiO<sub>2</sub>/sepiolite composites prepared at low temperature. *Chem Eng J* 2011;**173**:1–10. doi:10.1016/j.cej.2010.11.028.
- [13] Du YC, Stephanus A. Levenberg-marquardt neural network algorithm for degree of arteriovenous fistula stenosis classification using a dual optical photoplethysmography sensor. *Sensors (Switzerland)* 2018;**18**. doi:10.3390/s18072322.
- [14] Zamaniyan A, Joda F, Behroozsarand A, Ebrahimi H. Application of artificial neural networks (ANN) for modeling of industrial hydrogen plant. *Int J Hydrogen Energy* 2013;**38**:6289–97. doi:10.1016/j.ijhydene.2013.02.136.
- [15] Bustillo A, Pimenov DY, Matuszewski M, Mikolajczyk T. Using artificial intelligence models for the prediction of surface wear based on surface isotropy levels. *Robot Comput Integr Manuf* 2018;**53**:215–27. doi:10.1016/j.rcim.2018.03.011.
- [16] Kayri M. Predictive Abilities of Bayesian Regularization and Levenberg–Marquardt Algorithms in Artificial Neural Networks: A Comparative Empirical Study on Social Data. *Math Comput Appl* 2016;**21**:20. doi:10.3390/mca21020020.

- [17] Shi J, Zhu Y, Khan F, Chen G. Application of Bayesian Regularization Artificial Neural Network in explosion risk analysis of fixed offshore platform. *J Loss Prev Process Ind* 2019;**57**:131–41. doi:10.1016/j.jlp.2018.10.009.
- [18] Griffin WO, Darsey JA. Artificial neural network prediction indicators of density functional theory metal hydride models. *Int J Hydrogen Energy* 2013;**38**:11920–9. doi:10.1016/j.ijhydene.2013.06.138.
- [19] Casey JG, Collier-Oxandale A, Hannigan M. Performance of artificial neural networks and linear models to quantify 4 trace gas species in an oil and gas production region with low-cost sensors. *Sensors Actuators B Chem* 2019;**283**:504–14. doi:https://doi.org/10.1016/j.snb.2018.12.049.