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APPLICATION OF ARTIFICIAL NEURAL NETWORKS IN MODELING AND OPTIMIZATION OF BIOFUELS PRODUCTION

PRIMENA VEŠTAČKIH NEURONSKIH MREŽA U MODELOVANJU I OPTIMIZACIJI PROIZVODNJE BIOGORIVA

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ABSTRACT

Artificial neural networks, the artificial intelligence systems that imitate functions of biological neurons, have been widely used in different areas due to their variety and ability to conform to specificities of different applications. When it comes to application of artificial neural networks in bioprocess modeling, their task usually represents prediction or forecasting the values of dependent variables (outputs) based on given values of independent variables (inputs). Although bioprocess model is the „black box" and remains unknown, which could represent the obstacle in bioprocess analysis, neural networks have shown better ability in prediction of bioprocess results comparing to other modeling methods, such as RSM (Response Surface Methodology) and mathematical modeling. Obtained model could be further used for bioprocess optimization, commonly performed using genetic algorithms. This study provides the review of the main characteristics and applications of artificial neural networks in modeling and optimization of biofuels (bioethanol, biogas and biohydrogen) production.

***Key words**: artificial neural network, genetic algorithm, bioethanol, biogas, hydrogen, RSM*

REZIME

Veštačke neuronske mreže, kao sistemi veštačke inteligencije koji oponašaju funkcije ljudskog mozga i bioloških neurona, nalaze sve veću primenu u različitim oblastima usled svoje raznovrsnosti i sposobnosti prilagođavanja određenoj nameni. Kada je u pitanju primena veštačkih neuronskih mreža u modelovanju bioprocesa, njihov zadatak u najvećem broju slučajeva predstavlja predviđanje ili prognoziranje vrednosti zavisnih promenljivih (izlaza) na osnovu poznatih vrednosti nezavisnih promenljivih (ulaza). Model bioprocesa uslovljen je strukturom neuronske mreže, koja obuhvata arhitekturu neuronske mreže (broj slojeva, broj neurona u svakom sloju i način povezivanja neurona), vrednosti sinaptičkih težina i odabrane aktivacione funkcije. Iako sam model bioprocesa predstavlja „crnu kutiju" i ostaje nepoznat, što može da predstavlja poteškoću u analizi bioprocesa, veštačke neuronske mreže su pokazale znatno bolju sposobnost modelovanja, to jest predviđanja rezultata bioprocesa u poređenju sa drugim metodima modelovanja, kao što su metodologija odzivne površine i matematičko modelovanje. Dobijeni model dalje može da se koristi za optimizaciju bioprocesa, koja se najščešće vrši primenom genetičkih algoritama. Genetički algoritmi koriste model bioprocesa kao ciljnu funkciju, a process optimizacije predstavlja minimizaciju ili maksimizaciju date ciljne funkcije. Ovaj rad daje pregled osnovnih karakteristika i primene veštačkih neuronskih mreža u modelovanju i optimizaciji biotehnoloških procesa proizvodnje biogoriva, sa posebnim osvrtom na procese proizvodnje bioetanola, biogasa i biovodonika.

***Ključne reči**: veštačka neuronska mreža, genetički algoritam, bioetanol, biogas, vodonik, metodologija odzivne površine.*

INTRODUCTION

Artificial neural networks (ANNs) represent artificial intelligence systems created with an aim to imitate functions of human brain and biological neurons and to be applied in solving different problems which require performing of complex cognitive operations. ANNs have been used in different areas, such as pattern classification, clustering/categorization, function approximation, prediction/forecasting, associative memory and control (*Jain et al., 1996*). Their wide application is enabled due to variety of neural network types and their adaptability to certain application. The most usually used neural networks are based on multilayer perceptron architecture. Neural network architecture significantly affects its performance and usually adapts to concrete problem's demands. One of the neural networks elementary traits is their ability to learn, i. e. generalization ability based on the experience that network acquires in the training process.

Recent advances in biofuels production require better understanding of bioprocesses for biofuels production from different raw materials, agro-industrial byproducts and waste streams, as well as possibility to predict the outcomes of these processes in terms of biofuels yield and substrate utilization (*Olsson, 2007*). Optimization of biofuels production processes is also important from the aspect of yield increase and bioprocess cost reduction. Neural networks could be used as a tool for biofuels production modeling and optimization. The aim of this work is the review of the application and basic characteristics of artificial neural networks in modeling and optimization of biofuels production processes.

MATERIAL AND METHOD

Artificial neural network architecture is defined by the number of layers, number of neurons in each layer, transfer function and by the type of the interconnections between neurons (feed-forward or recurrent networks). Neural network training represents network introduction to explicit problem related data and process in which neural network tends to adapt its parameters through input data processing and outputs generation, with an aim to reduce error in solving the given problem, i.e. reducing the error between existing data and network predicted outputs. Network training is being performed

until network outputs satisfy previously defined error criterion. Afterwards, it is essential to perform network performance testing/validation and to assess its success in solving the given problem. Neural network applicability in certain situation depends significantly on its generalization ability, as well as on input data quality and training process parameters (*Witek-Krowiak et al., 2014*). Application of neural networks in bioprocess modeling represents prediction of process dependent variables based on independent variables varying, with the possibility of their application in process monitoring and control systems. Depending on the applied software, obtained bioprocess model usually remains unknown ("black box") (*Jokić et al., 2011*), which could represent an obstacle in bioprocess analysis, however, artificial neural networks show great potential and many advantages comparing to traditional bioprocess modeling approaches. Neural network models could be further used for bioprocess optimization, which is commonly performed using genetic algorithms. Genetic algorithm optimization is based on biological principles of combining and inheritance of genetic material, as well as on evolutionary survival principles of the fittest under the given conditions. Optimization is performed by minimizing or maximizing the objective function, which represents, in this particular case, neural network model (*Pal et al., 2009*).

RESULTS AND DISCUSSION

Bioethanol production

Due to the great interest in production of bioethanol from different agroindustrial remains in the past decade (*Dželetović and Mihailović, 2011*), a large number of studies concerning the application of artificial neural networks and genetic algorithms in modeling and optimization of these bioprocesses, as well as in modeling and optimization of other biofuels' production processes, could be found in the literature (Table 1).

Pramanik *(Pramanik, 2004*) investigated application of artificial neural networks for the prediction of variables' values in batch fermenter for production of ethanol from grapes waste using *Saccharomyces cerevisiae*. In this research neural network model was based on feed-forward architecture, backpropagation algorithm and sigmoid transfer function. Two neural networks were employed for prediction of ethanol and cell mass concentration, with common inputs: pH, temperature and sugar concentration. Each network had two additional inputs: ethanol or biomass concentration at time *(t-1)* and at time *t*. Levenberg-Marquardt optimization technique was used for network improvement by minimization of sum of squared errors. Results of cell mass and ethanol concentration at time *(t+1)* predicted by neural networks are very similar to the experimental results. Average sum of squared errors of 0.001 satisfied error criterion, while maximal relative percentage errors were 1.9077 and 1.9000 for ethanol concentration and biomass, respectively, presenting very good agreement. The best prediction was obtained using neural network with two hidden layers containing 15 and 16 neurons, respectively.

Saraceno et al. (*Saraceno et al., 2010*) simulated fermentation of ricotta cheese whey for production of ethanol using hybrid neural model, obtained by coupling artificial neural network approach with mass balance equations for lactose (substrate), ethanol and biomass. Multilayer perceptron with feed-forward pyramidal architecture, with descending number of neurons from input to output layer, was used. Network inputs were temperature, pH, reactor stirring rate, initial lactose concentration and reaction time. Bayesian regularization was used for training, i.e. synaptic weights and biases assessment. Transfer function was hyperbolic tangential function, except in output layer, where linear transfer function was used. Comparison of experimental data to predictions of hybrid neural models showed excellent concurrence with unitary slope and correlation coefficient of 0.999. It has been proved that suggested approach gives satisfying results since developed hybrid models have been characterized with average percentage error less than 10 %, which represents the limit for determination

Table 1. Application of ANN and RSM in modeling of biofuels production

Study	ANN	Architecture	Transfer function	ANN modeling results	RSM modeling results
Bioethanol production					
Study	ANN	Architecture	Transfer function	ANN modeling results	RSM modeling results
Bioethanol production					
Study	ANN	Architecture	Transfer function	ANN modeling results	RSM modeling results
Bioethanol production					
Study	ANN	Architecture	Transfer function	ANN modeling results	RSM modeling results
Bioethanol production					
Biohydrogen production					
Wang and Wan, 2009	feed-forward MLP	3-4-1	sigmoid	ASER=5%, yield 360.5 mg/g	ASER=12.8%, yield 289.9 mg/g
Whiteman and Kana, 2014	MLP	4-6-10-1	sigmoid	R^2=0.91, PE=15.12%	R^2=0.75, PE=19.08%
El-Shafie, 2014	MLP	3-6-4-2-1	sigmoid, linear	PE<10%, R^2=0.984	R^2=0.895
Biogas production					
Kanat and Saral, 2009	MLP	4-4-2	sigmoid	model successfully estimated biogas production rate	
Fakharudin et al., 2013	MLP			ASE=0.0002, yield 1.9583 g/L	ASE=0.0005, yield 1.9497 g/L
Dach et al., 2015	MLP	bovine slurry 5-11-1, porcine slurry 5-7-1		ρ=0.99	

MLP – multilayer perceptron; RPE – relative percentage error; APE – average percentage error, ρ – correlation coefficient; R^2 – coefficient of determination; ASER – average squared error root, PE – prediction error; ASE – average squared error

of model reliability. It has been also important to notice that hybrid neural models had showed lower average percentage error comparing to neural network model.

Jokić et al. (*Jokić et al., 2012*) investigated production of bioethanol in batch process using suspended *Saccharomyces cerevisae* cells from thick juice which was obtained as intermediate product of sugar beet processing. Non-recurrent neural network with one hidden layer and hyperbolic tangential transfer function was used. Input variables were initial sugar content and fermentation time, while output variables were yeast cells number, ethanol content and sugar content. Established optimal network topology was 2-9-1. Obtained coefficients of determination values, which were 0.9997, 0.9997 and 0.9999 for ethanol content, yeast cells number and sugar content, respectively, suggested very good agreement with experimental data in the chosen range of initial sugar content and fermentation time, and these values were better comparing to the values for models obtained by RSM modeling (0.938, 0.894 and 0.968, respectively) (*Grahovac et al., 2012a*). Study reported by Jokić et al. (*Jokić et al., 2011*) investigated effects of independent variables to the network outputs, under the same conditions, using Garson's algorithm and synaptic weights method. It has been found that fermentation prolongation progressively increases ethanol content, as well as yeast cells number, therefore, it has excitatory effect, while it shows inhibitory effect to sugar content. On the other hand, increase of initial sugar content positively affects all chosen neural network outputs.

Bioethanol can be produced from different byproducts and waste materials (*Mojović et al., 2010*), for example, using different intermediates from sugar beet processing (*Grahovac et al., 2011*). Grahovac et al. *(Grahovac et al., 2012b*) studied effects of input variables (substrate type – raw, thin, thick sugar beet juice and molasses) and fermentation time to output variables (ethanol content, yeast cells number and sugar content) during batch fermentation using different starter cultures. Application of different *Saccharomyces cerevisiae* strains in bioethanol production was previously investigated (*Ranković et al., 2009*). A feed-forward back-propagation artificial neural network was applied in this study. Neural network training was carried out using Levenberg-Marquardt algorithm, while transfer function was hyperbolic tangential function. For each starter culture, optimal network topologies for ethanol content and yeast cells number were 2-7-1, while 2-10-1 was optimal network topology for residual sugar content. For all strains cumulatively, optimal network topology for ethanol content was 3-9-1, while optimal network topologies for yeast cells number and residual sugar content were 3-11-1. Obtained coefficients of determination for network used for ethanol content prediction (3-9-1 and 2-7-1) were 0.9982 and 0.9999, respectively. When it comes to yeast cells number, coefficients of determination were 0.9996 (network 2-7-1) and 0.9909 (network 3-11-1). During determination of residual sugar content, coefficients of determination were 0.9999 and 0.9992, for networks 2-10-1 and 3-11-1, respectively. In all examined cases, neural networks have shown good ability of output variables prediction.

Oilseed rape straw has been used as a low-cost substrate for ethanol production. The effect of steam explosion to chemical composition, enzymatic hydrolysis and simultaneous saccharification and fermentation (SSF) was examined (*Talebnia et al., 2015*). Considering different reaction mechanisms involved in hydrolysis and SSF, separate neural networks were developed for each step. For hydrolysis step developed network was feed-forward multilayer perceptron with two hidden layers consisting of 5 and 6 neurons. Network inputs were solid phase mass, pretreatment temperature, pretreatment duration, acid concentration and reaction time, while outputs were glucose and xylose concentrations. Due to simultaneous production and consumption of sugar and relationship between glucose consumption and ethanol production in SSF phase, developed network represented combination of feed-forward and recurrent network, consisting of 3 layers, where hidden layer contained 16 neurons. Glucose and xylose concentrations obtained after hydrolysis pretreatment and reaction time were set as input variables, while network outputs were concentrations of glucose, xylose and ethanol during fermentation. Backpropagation algorithm was used for network training, and transfer function was hyperbolic tangent sigmoid function. Models should have predicted concentrations of these three substances during process course, i.e. reaction time which was 0-48 h for hydrolysis and 0-72 h for SSF. For two sets of tested data values of determination coefficient and average squared error were 0.837, 0.0061 and 0.961, 0.0017, respectively. Developed models have showed good prediction ability for glucose and ethanol concentrations, while their prediction ability for xylose concentration was lower because xylose concentration remains almost constant during process due to inability of yeast to consume it. For modeling of an entire process two networks were combined and united network was considered as a model for process control. Two outputs of the first network (glucose and xylose concentrations after hydrolysis) and fermentation time were set as input variables for the second network. Values of coefficients of determination were 0.9829, 0.9086 and 0.9979 for glucose, xylose and ethanol concentrations, respectively, which confirmed that model based on artificial neural network could represent reliable method for modeling of bioprocesses such as enzymatic hydrolysis and SSF.

The aim of the study reported by Grahovac et al. (*Grahovac et al., 2016*) was modeling of the bioprocess for production of bioethanol from intermediates and byproducts of sugar beet processing using artificial neural networks based on multilayer perceptron architecture. Prediction of fermentation of each substrate using neural network had the same input variables (fermentation time and initial sugar content) and one output variable (ethanol content, yeast cells number or sugar content), while transfer function was hyperbolic tangential function. Results showed that appropriate model could be obtained using networks with one hidden layer. Neural network with the best prediction results for outputs of raw or thin juice fermentation contained 8 neurons in the hidden layer for all selected outputs. On the other hand, optimal numbers of neurons in hidden layer for thick juice and molasses fermentation were 8 and 9, respectively. After assembling data for all substrates, additional input (substrate type) was added and optimal network architecture for each output was 3-12-1. Obtained results suggested that artificial neural networks represent appropriate tool for prediction of chosen network outputs, with correlation coefficient of 0.999. On the other hand, kinetic modeling of raw juice batch fermentation has showed lower accuracy comparing to neural network models, with correlation coefficient of 0.997 (*Dodić et al., 2012*). Modeling of bioethanol production from raw sugar beet juice using RSM is characterized by correlation coefficients of 0.928, 0.962 and 0.965 for cells number, ethanol yield and fermentable sugar content, respectively (*Popov et al., 2010*), which implies better modeling ability of applied neural network models.

Biohydrogen production

Wang and Wan (*Wang and Wan, 2009*) applied central composite design to explore the effect of temperature, initial pH and glucose concentration to fermentative production of biohydrogen by mixed culture in batch bioprocess. Comparison

of modeling ability of RSM and neural network was carried out, as well as comparison of optimization ability of RSM and neural network based genetic algorithm, whose purpose is optimization of biohydrogen yield. Neural network with feed forward architecture, backpropagation training algorithm, sigmoid transfer function and topology 3-4-1 was used, where output variable was biohydrogen yield. Average square error root value (12.8 %) for RSM model was significantly larger than the value for neural network model (5 %), implying that neural network model has showed better modeling ability than RSM. Maximal biohydrogen yield of 289.9 mL/g glucose which was identified using RSM was lower than the yield obtained using genetic algorithm based on neural network model (360.5 mL/g glucose), suggesting that the latter shows better optimization capacity than RSM.

Study reported by Whiteman and Kana (*Whiteman and Kana, 2014*) comparatively assess modeling efficacy of biohydrogen production using RSM and artificial neural network. Input parameters were molasses concentration, pH, temperature and inoculum concentration. Neural network had 4-6-10-1 topology, multilayer perceptron structure and sigmoid transfer function. Coefficient of determination values for RSM and neural network were 0.75 and 0.91, respectively. After validation, prediction error of 15.12 % for neural network and 19.08 % for RSM were noticed. These results point out that neural network has showed higher accuracy for modeling of relationships between considered process parameters during fermentative biohydrogen production and therefore it is more reliable for navigation in the optimization space.

Potential of neural network model application for simulation and prediction of biohydrogen yield in batch process using *Clostridium saccharoperbutylacetonicum* N1-4 (ATCC 13564) was investigated in research conducted by El-Shafie (*El-Shafie, 2014*). Unique network architecture (3-6-4-2-1), based on multilayer perceptron structure, that imitates relationships between 3 input parameters (initial substrate content – glucose, initial pH and temperature) was introduced. Sigmoid and linear transfer function in its first and second layer, respectively, were used. Results showed that the prediction error of neural network model was lower than 10 %. Neural network provided higher accuracy for prediction of biohydrogen yield with coefficient of determination of 0.984 comparing to the Box-Vilson design (coefficient of determination 0.895), under the same conditions. Suggested model based on neural network reliably predicts biohydrogen yield and could be further used as predictive controller for fermentative system for biohydrogen production at industrial scale.

Biogas production

Biogas production rate was modeled and estimated in thermophilic UASB (Upflow Anaerobic Sludge Blanket) reactor (*Kanat and Saral, 2009*). Experimental data cover stationary state period and period of unusual process conditions – organic substrate addition. The half of the experimental data was used for network training, and the other half was used for model testing. Neural network with multilayer perceptron structure, backpropagation training algorithm and sigmoid transfer function was applied, and its architecture was 4-4-2. Network inputs were organic loading rate, total volatile fatty acid of the effluent, influent–effluent alkalinity, influent–effluent pH, and temperature of the reactor. Using the trends of estimated data a conclusion can be made that model successfully estimated biogas production rate during stationary state conditions, while results in organic load periods were successfully followed. Neural network models gave encouraging estimation results for on-line control of thermophilic reactors.

Study reported by Fakharudin et al. (*Fakharudin et al., 2013*) has suggested the frame for modeling of biogas production using artificial neural networks and biogas yield optimization using genetic algorithms. Neural network was based on multilayer perceptron structure, and input variables were temperature, hydraulic retention time and organic loading rate. Neural network model accuracy was high with average squared error of 0.0002, comparing to RSM (average squared error 0.0005). Results have showed that precise modeling with low error does not provide much higher yield. Neural network model trained using backpropagation algorithm, with 5 hidden neurons, has predicted maximal biogas yield of 1.9583 g/L, which represents the increase of 0.44 % comparing to maximal biogas yield obtained using RSM model (1.9497 g/L).

Research conducted by Dach et al. (*Dach et al., 2016*) aimed at development of neural network model for prediction of methane emission during slurry fermentation. Slurry fermentation provides its deodorization and significantly affects sanitation process. Input variables were day of measurement, slurry dry matter, organic slurry dry matter, pH and conductivity. Output variable was accumulated methane content. Optimal choice for bovine slurry fermentation was the network with 5-11-1 architecture, while 5-7-1 network architecture was optimal for porcine slurry fermentation. Both neural networks had multilayer perceptron structure. Correlation coefficients were very high (0.99) for both neural network models, proving high correlation between results obtained using neural networks and the experimental data. This suggests suitability of generated neural networks as instruments for prediction of methane content obtained by bovine and porcine slurry fermentation.

CONCLUSION

Artificial neural networks have shown superiority over conventional modeling methods, such as regression analysis, mathematical modeling and RSM, in terms of accuracy of predicting process output variables. Application of genetic algorithms in many cases has led to increase of desired component yield under the optimized process conditions. The review of literature data revealed an increasing trend of application of neural networks in modeling and optimization of biofuels production processes, which is expected to continue in the following years, considering the potential of its application in solving prediction and control problems in different biotechnology areas.

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