

Neural network simulation in running of acetic acid synthesis unit while start-up

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Summary. The present article focuses on the researches' results of artificial neural networks architecturing using in automated control systems for acetic acid synthesis unit by means of GUI, i.e. Neutral Network Toolbox interface of the software simulator Matlab. The structural schemes of such systems are attached.

Key words: neural network with feed-forward back propagation; radial-basic neural network; activation function.

INTRODUCTION

To run complex systems, it is necessary to build a model adequately reflecting the properties of the object to be controlled. In the majority of cases such model parameters are determined directly within the process of object is in operation, i.e. the identification is performed on the basis of occasional input and output signals. Nowadays the way of automated control systems architecturing on the basis of artificial intelligence technologies usage (e.g. neural networks, fuzzy logic, genetic algorithms) [6, 8, 11-14, 17, 29, 30] is being rapidly developed. Those factors which are badly formalized using common mathematical methods may be subjected to generalization (e.g. one's professional experience or intuition, etc.). Only few attempts are known to use artificial intelligence technologies in chemical industry. They are used to interpret sensors' readings, to run temperature mode of the technological processes, to monitor chemical and technological processes [1-5, 7, 9, 10, 15, 16, 18-28].

Architecturing and researching of artificial neural networks performance can be carried out via software-based simulators. The most commonly used packages to model neural networks characteristics are as follows: Neural Works Pro Plus, Neuro Solution, Matlab (Neural Network Toolbox), Neuro Wisard, ANsim, Neural Ware and others. The software is differed by its complexity, quantity of neurons types and algorithms of studying maintained at the system.

MATERIALS AND METHODS

The purpose of the present work was the building up and researching of the neural network properties which might be used in running of acetic acid synthesis unit at start-up at PJSC "SEVERODONETSK AZOT ASSOCIATION". For this purpose the statistical data of the acetic acid synthesis unit while the plant starting up process were used. Block diagram of the column acetic acid synthesis is shown in figure 1.

Analysis of the acetic acid synthesis unit as a control object shows that concentration Q of acetic acid, process temperature T , pressure P in the synthesis column and the reaction mass level L in the reactor may be used as the output coordinates.

To control the synthesis column as control (input) coordinates can be used the flow rate of methanol F_1 and carbon monoxide F_2 fed to the reactor .

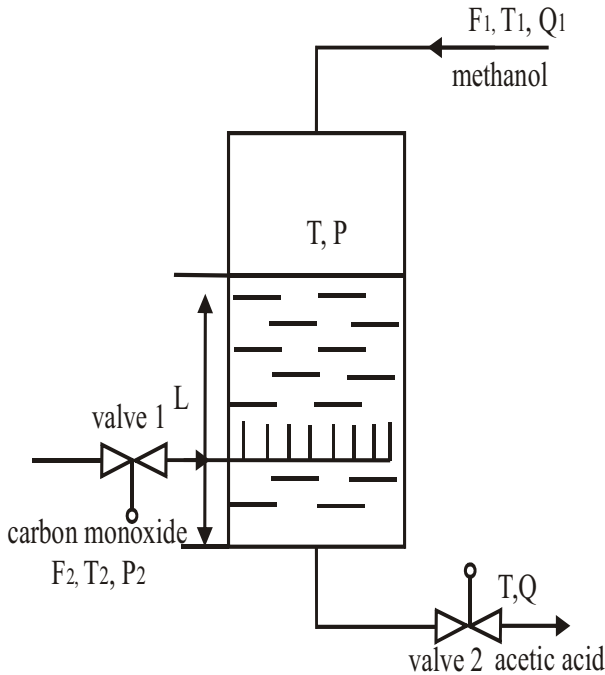


Fig. 1. Block diagram of the column for synthesizing acetic acid

All other parameters of the process: the temperature of the methanol feed T_1 , supply pressure of carbon monoxide P_2 , the temperature of the feed carbon monoxide T_2 , should be attributed to the perturbing parameters.

Information and logic synthesis column acetic acid is shown in figure 2.

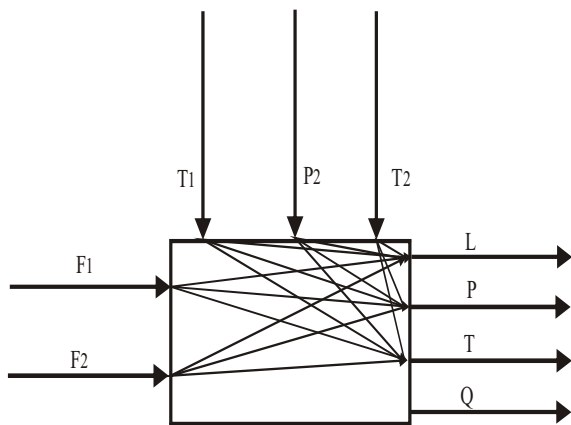


Fig. 2. Information and logic diagram synthesis column acetic acid

The environment of software-based simulator MATLAB 7.1.0 (GUI - Neural Network Toolbox interface) was used for building up process. This pack is recommended for neural network with different type of activation function architecturing.

The following parameters were used as the input data:

1. Inlet methanol consumption.
2. Inlet carbon oxide consumption.
3. Inlet methanol temperature.
4. Inlet carbon oxide pressure.
5. Inlet carbon oxide temperature.

The following parameters were used as the output data:

1. Reaction mass level at the unit.
2. Reaction mass pressure at the unit.
3. Reaction mass temperature at the unit.

50% of the main observations were involved in the process of the neural network learning (the other half was used for verification purposes).

RESULTS

The structure and parameters of the neural network with feed-forward back propagation shown at Fig.3 were determined as a result of GUI - Neural Network Toolbox interface MATLAB 7.1.0.

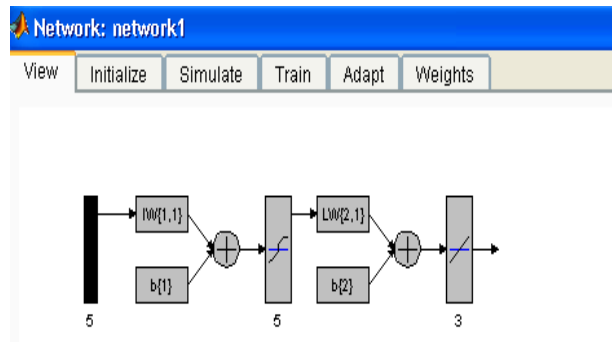


Fig. 3. Neural network with feed-forward back propagation structure

The network was built up on the basis of five neurons at the network input, five sigmoid (TANSIG) neurons of a buried layer and three linear (PURELIN) neurons of an output layer. The functions implementing learning algorithm as well as training and error functions ensuring minimum relative accuracy of data approximation were determined to build up the network. The respective parameters of three networks for the acetic acid synthesis units are given in tab. 1.

While making a comparison of the networks respective parameters, the following observations were found: the minimum relative accuracy is insured by the network based on gradient descent method with disturbance as a learning function, function of the gradient descent with account of the moments as a training function, mean-square error as an error function.

Table 1. Neural networks parameters with feed-forward back propogation

Net-work Number	Learning algorithm implementing function	Training function	Error function	Output parameter	Relative accuracy	Average relative accuracy
1	2	3	4	5	6	7
1	Gradient descent method	Learning function of gradient descent with account of the moments	Mean-square error	1	0,078	0,075
				2	0,060	
				3	0,086	
2	Gradient descent method with account of the moments	Learning function of gradient descent	Mean-square error	1	0,790	0,312
				2	0,061	
				3	0,086	
3	Levenberg-Marquardt method	Learning function of gradient descent	Mean-square error	1	0,801	0,316
				2	0,062	
				3	0,086	

In addition, a radial-basic neural network which structure is shown at fig.4 was built up as a result of the research.

The parameters of the input \bar{P} and target values \bar{T} arrays, as well as GOAL (network tolerated mean-square error) and SPREAD parameters (the parameter of interference) were used as the input data for the radial-basic networks, while radial-basic network parameters were used as output data. SPREAD parameter of interference was taken to be bigger than a partition step of the learning sequence interval, but smaller than the interval itself, that is equal to 0.1. GOAL parameter was chosen to be equal to 0. While architecturing of the radial-basic network with a zero error, the number of neurons of a radial-basic layer is equal to the number of input values. Weight and bias of the radial-basic network are set in such a way that its outputs are accurately equal to the targets. Relative accuracies of the data fitting were determined as a result of networks forecasting by means of a testing data selection. The respective parameters of the network with a minimum relative accuracy for acetic acid synthesis unit are given in tab. 2.

If we compare the relative accuracies of feed-forward neural networks to those of a radial-basic network, we can see that the minimum relative accuracy is insured by the radial-basic neural network, that is one of the networks has an

advantage before another in solution of the management problem. There're much more neurons in the radial-basic networks than a compared network with feed forward signal and sigmoid activation functions at a buried layer has.

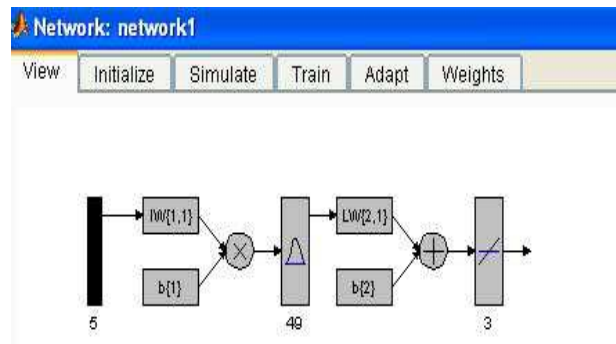


Fig. 4. Radial-basic network structure

Table 2. Radial-basic neural network parameters

Interference parameter	Mean-square error	Output parameter	Relative accuracy	Average relative accuracy
1,0	0	1	0,025	0,016
		2	0,002	
		3	0,020	

CONCLUSIONS

To create control system with the usage of the neuron networks at the acetic acid synthesis unit start-up process it's necessary to determine neuron network structure, to hold a learning on the basis of technological specifications and to do the approbation of network performance with an application of acetic acid plant equipment. Neural network architecting with a usage of GUI - Neural Network Toolbox interface MATLAB 7.1.0 has proved the success of the neuron network building up and learning process and its satisfactory quality. That will let use neural networks to manage the technological processes of the acetic acid synthesis and proves the urgency of the further researches of this area.

REFERENCES

1. **Afanasenko A.G., Verevkin A.P., 2009.:** Neuronet simulation of carbonation process quality rating. *Vestnik U.*, Vol. 13 №2 (35), 222-225.
2. **Baskin I.I., Palyulin V.A., Zefirov N.S., 2006.:** Multilayered perceptrons in "structure-property" relationship studies for organic compounds. *Rus. Chem. Journ.* (Journal of Russian chemical society after D. I. Mendeleev), T. L. №2., 86-96.
3. **Baskin I.I., Palyulin V.A., Zefirov N.S., 2005.:** Using artificial neural networks for chemical compounds properties prognostication. *Neural computers: design, applications*, № 1-2, 98-101.
4. **Baskin I.I., Skvortsova M.I., Palyulin V.A., Zefirov N.S., 1997.:** Quantitative chemical structure-property/activity relationship studies using artificial neural networks. *Foundations of computing and decision sciences*. Vol. 22, №2, 107-116.
5. **De Souza, M. B., Pinto J. C., et al., 1996.:** Control of a chaotic polymerization reactor: A neural network based model predictive approach. *Polymer Engineering and Science*, 36(4), 448-457.
6. **Galushkin A.I., 2000.:** The book. *Theory of neural networks*. M.: I, 416.
7. **Gardner J.W., Hines E.L., Wilkinson M., 1990.:** Application of artificial neural networks to an electronic olfactory system. *Measurement science and technology*. Vol. 1, 446-451.
8. **Haykin S., 2006.:** The book, *Neural networks. Complete course*. M.: Williams, 1104.
9. **Hong H.-K., Kwon C.N., Kim S.-R., 2000.:** Portable electronic nose system with gas sensor array and artificial neural network. *Sensors and Actuators B.*, Vol. 66, 49-52.
10. **Huang, Y. F., G. H. Huang, et al., 2003.:** Development of an artificial neural network model for predicting minimum miscibility pressure in CO₂ flooding. *Journal of Petroleum Science and Engineering*, 37(1-2), 83-95.
11. **Karimov R.N., 2000.:** Experimental information processing. P.3. *Multivariate analysis: learning aid*, Saratov: SSTU, 108.
12. **Kruglov V.V., Borisov V.V., 2002.:** The book *Artificial neural networks. Theory and practice*. 2nd edition, pattern, M.: Hot line – Telecom, 382.
13. **Kruglov V.V., Borisov V.V., 2001.:** The book, *Hybrid neural networks.*, Smolensk: Rusich, 224.
14. **Kusz A., Maksym P., Marciniak A.W., 2011.:** Bayesian networks as knowledge representation system in domain of reliability engineering. *TEKA Commission of Motorization I Energ. Roln.*, 11 C, 173-180.
15. **Larachi F., 2001.:** Neural network kinetic prediction of coke burn-off on spent MnO₂/CeO₂ wet oxidation catalysts. *Applied Catalysis B, Environmental*, 30(1-2), 141-150.
16. **Larachi F. and Granjean B. P. A., 2000.:** Comments on "Neural network modeling of structured packing height equivalent to a theoretical plate" and "HETP and pressure drop prediction for structured packing distillation columns using a neural network". *Industrial & Engineering Chemistry Research*, 39(11), 4437-4437.
17. **Medvedev V.S., Potemkin V.G., 2002.:** The book, *Neural networks. MATLAB 6*. Under the editorship of Cand. of Sc. Potemkin V.G., M.: DIALOG IEFI, 495.
18. **Nagy Z., American Institute of Chemical Engineers., et al., 2000.:** A Comparison of First Principles and Neural Network Model Based Nonlinear Predictive Control of a Distillation Column. Distributed by American Institute of Chemical Engineers, New York, *N.Y.*
19. **Park J.-K., 1993.:** Modeling of Distillation Column and Reactor Dynamics Using Artificial Neural Networks (*Neural Networks*). *DAI-* 55, №., 01B, 6660.
20. **Sabharwal A., 1998.:** A Hybrid Approach Applied to an Industrial Distillation Column That Compares Physical and Neural Network Modeling Techniques. *MAI*, 37, no. 02, 0648.
21. **Santos V. M. L., Carvalho F. R., et al., 2000.:** Predictive control based on neural networks: An application to a fluid catalytic cracking industrial unit. *Brazilian Journal of Chemical Engineering*, 17(4-7), 897-905.
22. **Su G. H., Fukuda K., et al. 2002.:** Application of an artificial neural network in reactor thermohydraulic problem: Prediction of critical heat flux. *Journal of Nuclear Science and Technology*, 39(5), 564-571.
23. **Su G. H., Fukuda K., et al. 2002.:** Applications of artificial neural network for the prediction of flow boiling curves. *Journal of Nuclear Science and Technology*, 39(11), 1190-1198.

24. **Su C., Hino J., et al. 2000.:** Prediction of chatter in high-speed milling by means of fuzzy neural networks. *International Journal of Systems Science* , 31(10), 1323-1330.
25. **Sysoyev V.V., Musatov V.J., Silayev A.V., Zaliyalov T.R., Maschenko A.A., 2007.:** The application of neural networks method for response analysis of the gas identification multisensory system-on-chip. *Bulletin of Saratov State Technical University, №1 (21), issue 1, 80-87.*
26. **Topolski N.G., Vatagin V.S., 2000.:** Computer-aided fire safety systems in chemical industries. *Mary Kay O'Connor Process safety center symposium. Proceeding. October 24-25, Reed Arena, Texas A&M, University, College Station, Texas, 348-349.*
27. **Vatagin V.S., Nevsky A.V., 2005.:** Neurotechnologies of designing integrated automated control systems of industrial safety. *State-of-the-art high technologies, vol. 4, 75-81.*
28. **Zhang H., Balaban M.O., Principe J.C., 2003.:** Improving pattern recognition of electronic nose data with time-delay neural networks. *Sensors and Actuators B., Vol. 96, 385-389.*
29. **Ossovsky S. 2002.:** Neural networks for data processing .Translation from Polish by Rudinsky. *M.: Finances and statistics, 304.*
30. **Ulshin V., Yurkov D. 2010.:** The adaptive system on the basis of artificial neuron networks. *ТЕКА Commission of Motorization I Energ. Roln., 10 D, 15-24.*

НЕЙРОСЕТЕВОЕ МОДЕЛИРОВАНИЕ
ДЛЯ УПРАВЛЕНИЯ КОЛОННОЙ СИНТЕЗА
УКСУСНОЙ КИСЛОТЫ В ПЕРИОД ПУСКА

Ольга Поркуян, Жанна Самойлова

Аннотация. В данной статье приведены результаты исследований построения искусственных нейронных сетей, используемых в автоматизированных системах управления колонной синтеза уксусной кислоты с помощью GUI –интерфейса Neural Network Toolbox программного симулятора Matlab. Приведены структурные схемы подобных сетей.
Ключевые слова: нейронная сеть с обратным распространением ошибки, радиально-базисная нейронная сеть, функция активации.