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Abstract. An artificial neural multi-layer network has been developed for predicting the mass transfer coefficients in the liquid and gas phases for the gas absorption (CO2) from the air using an absorbent - water. For the development of neural network the unobservable parameters of the packed absorber were calculated. The obtained results can be used to model an extensive class of chemical engineering processes with the possibility of formalizing the calculation procedures.

The approaches to solving the applied problems of chemical technology evolve at the level of understanding the principles of the computation process organization. If the traditional methods are the operations with numbers and symbols, specialized in any specific algorithm, then the neural network modeling, a direction for the development of computational mathematics, operates with nonformalized algorithms, which are found by the neural networks. The growing importance of neural network modeling is due to the growing level of complexity of the modern chemical-technological systems and the need for the detailed mathematical description [1-3].

The research related to the use of neural networks for solving the applied problems is being conducted in various scientific areas. In chemistry, physical chemistry and chemical technology, the artificial neural networks are most often used for prediction [4–7], modeling [8, 9], control and decision making [10], also for data analysis [11, 12], classification [13] and optimization [14,15].

The neural network approach in solving the problems has advantages in the following cases: 1) there is no problem formalization, since it contains the elements of uncertainty; 2) the problem formalization is present, but there is no mathematical apparatus for its solution; 3) the problem formalization is present, the mathematical apparatus is present, but its implementation is laborious and leads to a simplification of the algorithms and reduces the quality of solutions.

The purpose of this study is to develop an artificial neural multi-layer network of direct distribution, which will determine the mass transfer coefficients in the liquid and gas phases (as an example of the process of gas absorption (CO2) from the air by the absorbent - water).

The unobservable parameters of the packed absorber were calculated. The developed neural network calculates the mass transfer coefficients for the gas and liquid phases when the device operates in a stationary mode.

For the implementation of an artificial neural network, the AForge.NET framework was chosen when calculating the mass transfer coefficients. For training and testing of neural networks, the sets of training and testing pairs of vectors are formed, to define input and output variables (table 1).

Table 1. Input and output parameters of the neural network.

Input	Output
Initial Absorbate Concentration, y_i	Liquid-Phase Mass-Transfer Coefficient, β_l
Final Absorbate Concentration, y_f	
Volume Flow Rate, V_0	Gas-Phase Mass-Transfer Coefficient, β_g
Water Temperature, t	
Absorbate Pressure, P	

The training and test data samples were compiled from the experimental data. The neural network training is more effective when normalization of input and output variables is performed, which was done before the start of the training process. The normally distributed random numbers in the range from 0 to 1 were chosen as the normalized variables of the input variables.

The architecture of an artificial neural network is as follows: the network will have five neurons in the input layer, ten in the hidden layer and two in the output layer (network 5-10-2) (Figure 1).

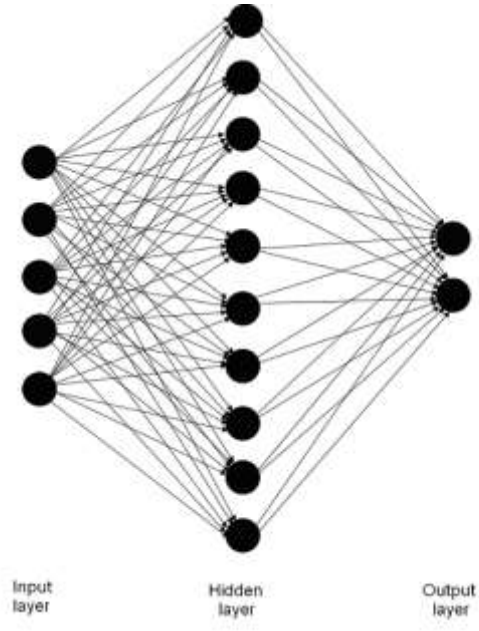

Figure 1. Neural network topology.

The training and testing vectors are formed from a variety of input and output data. The testing pairs are presented in table 2.

Table 2. Test sample.

Input Vector						Output Vector	
№	V_0	Y_i	Y_f	T	P	$\beta_g 10^2$	$\beta_l 10^6$
1	7.1	8.3	0.8	61.4	12.9	0.592485704068183	5.2598494621728
2	7.3	9.7	0.9	56.6	13.8	0.579046014257464	4.8150089875848
3	6.7	9	0.8	50.7	12.7	0.639772079982268	5.1676781157875
4	7.2	9.7	0.6	68.2	11.1	0.611736241326955	6.4204309723738
5	5.3	8.4	0.7	66.3	14.2	0.534263380473983	4.8078357094432
6	6.9	8.1	0.7	67.8	10.4	0.654684082129212	6.8477735140176
7	5.2	7.8	0.8	54.8	14.4	0.578865419035652	4.5312867022008
8	6.1	9.8	0.8	56.7	13.6	0.580859585765781	4.9080613293260
9	7.2	7.3	0.7	57	12.7	0.620110224152713	5.2618179912281
10	6.1	7.8	1	53.1	11	0.711283726312683	6.0633595466088

The optimal number of neurons in the hidden layer is determined by the formula [16], which is equal to 11, therefore, in table 3, their number closest to the optimum is equal to 10.

Table 3. Hidden layer W1.

№	I=1	I=2	I=3	I=4	I=5
1.	0.025027	0.037251	-0.019779	-0.008142	1.159427
2.	0.367376	1.104361	0.4181876	0.6184764	0.810058
3.	-0.312330	0.215481	0.3601997	0.8885924	0.436505
4.	0.9416578	1.229107	0.8627509	0.5235855	0.656929
5.	0.0016111	0.464742	-0.658497	2.0142734	0.366389
6.	0.4622430	0.824699	0.144913	0.788472	0.712788
7.	0.1692568	1.097325	1.140483	1.054402	0.577029
8.	-0.048560	0.213767	-0.129379	1.889137	-0.572945
9.	-0.133689	-0.078429	-0.117341	-0.405655	9.3679517

10.	-0.545761	-0.263469	0.277923	4.376352	5.2733550

Table 4. Output layer W2.

№	j=1	j=2
1	-4.125341	-3.358782
2	0.9945531	1.1141421
3	0.6250765	-0.142361
4	1.3250474	0.9671626
5	1.8854393	0.6080750
6	0.3109761	-0.174296
7	1.7836284	1.1951391
8	-2.082939	0.3702943
9	-2.256111	-5.2937988
10	-3.221286	-5.2937988

For network training, the results were set at a relative error of 0.5%. The weight coefficients are presented in table 3,4.

In order to select the architecture of an artificial neural network, the deviations of the calculated values of the mass transfer coefficients of the gas and liquid phases from the experimental values were determined (table 5). The most optimal architecture of an artificial neural network is the architecture 5-10-2, which gives the smallest deviation in β_l, β_g.

Table 5. Input and output parameters of the neural network.

Architecture	Error β_g	Error β_l
5-5-2	$4.74752*10^{-5}$	$8.11155*10^{-7}$
5-6-2	$5.74983*10^{-5}$	$6.36088*10^{-7}$
5-7-2	$4.70527*10^{-5}$	$7.4511*10^{-7}$
5-8-2	$6.50883*10^{-5}$	$8.27173*10^{-7}$
5-9-2	$6.68836*10^{-5}$	$9.02349*10^{-7}$
5-10-2	$4.59501*10^{-5}$	$7.14545*10^{-7}$
5-11-2	$5.35965*10^{-7}$	$8.31043*10^{-7}$

The test adequacy of the neural network to the experiment is checked using the Fisher test, since it is assumed that the dispersions for the mass transfer coefficients are independent. After training, the responses of the neural network to the testing effects, which were used to test the adequacy of the neural network to the experiment, were calculated.

Table 6. Fisher test.

Test	β_g	β_l
RMS Model Difference	0.00027	0.00044
RMS Experiment Difference	0.00011	0.00056
Fisher Test, F	2.454	0.785

For f=9, at a significance level of 0.05, Fisher test $F_т$ is equal to 3.169. Since $F < F_т$, the model is adequate for the process.

The artificial neural network was implemented in the C# language in the Visual Studio development environment using the A Forge Neuro library. In the course of work, a full-fledged Windows Forms application was created. The functions of loading the training sample from a file, setting the required accuracy of training, and entering the vector to obtain the results of the neural network were performed in it. .

The keyboard input was verified, while the user had the opportunity to enter only numbers and separator symbols, and the points were automatically replaced with binary commas for the convenience of data recording in the program. An interface was also implemented for calculating the theoretical values of the mass transfer coefficients using known algorithms [17].

An application for predicting the mass transfer coefficients of the absorption process using artificial neural networks has been developed. The training and test network samples were compiled using experimental data, and the responses of the neural network were obtained. Thus, using the multilayer neural networks, a neural model of interaction between the technological factors and process intensity indices was developed.

References

[1] Aminova G A, Manuyko G V, Ignashina T V, Bronskaya V V , Kharitonova N E, Dyakonov G S and Arkhireev V P 2006 Optimum Parameters of Butadiene Polymerization during the Rubber Synthesis on a Neodymium-Containing Catalytic System *Theoretical Foundations of Chemistry Technology* **40** 63-71

[2] Manuyko G V, Aminova G A, Bronskaya V V, Ignashina T V, Dyakonov G S and Bashkirov D V. 2008 Calculation of the Molecular Mass Distribution of the Polymer Obtained in the Cascade of Reactors, Taking into Account Chain Transfer to Polymer T*heoretical Foundations of Chemical Technology* **42** 348-51

[3] Aminova G A, Manuyko G V, Bronskaya V V, Ismagilova A I and Dyakonov G S 2005 Mathematical modeling of butadiene rubber synthesis process on neodymium-containing catalyst system *Polymer Science – Series A* **48** 881-6

[4] Amiri Sahar et al. 2011 An artificial neural network for prediction of gas holdup in bubble columns with oily solutions *Neural Comput. and Appl.* **20** 487-94

[5] Albaugh Daniel R et al. 2009 Prediction of HPLC retention index using artificia neural networks and IGroup E-state indices *J. Chem. Inf. and Model.* **49** 788-99

[6] Tumanov V E 2010 Use of an Artificial Neural Network to Predict the Reactivity of Molecules in Radical Reactions *Inf. Tehnol.* **5** 11-5

[7] Popok N I, Pyata M V 2008 Using Neural Networks and Fuzzy Logic to Predict the Physicochemical Properties of Materials *Polzunovsky Vestnik No. 1-2*

[8] Zgoul Moudar H 2012 Use of artificial neural networks for modelling rate dependent behaviour of adhesive materials *Int. J. Adhes. and Adhes.* **36** 1-7

[9] Mirzaei E et al. 2012 Artificial neural networks modeling of electrospinning of polyethylene oxide from aqueous acid acetic solution *J. Appl. Polym. Sci.* **125** 1910- 21
[10] Sletnev M S 2010 Software Development of a Decision Support System for Managing Technological Plants for the Production of Ethylene and Propylene on the Basis of Neural Network Technologies *Collection of works of the All-Russian Scientific and Technical Conference dedicated to the 50th anniversary of the Automation of Technological Processes and Production department of Ufa State Petroleum Technical University* 89-92
[11] Gotovtsev P M et al. 2008 Analysis of the Coolant State using Artificial Neural Network *Heat Power Industry* **7** 15-20
[12] Wang Bin et al. 2009 Quantitative analysis of diclofenac sodium powder via nearinfrared spectroscopy combined with artificial neural network *J. Pharm. and Biomed. Anal.* **50** 158-63
[13] Charhyia Nadir Nizar and Dudul Sanjay Vasant Ali 2008 Sensor for classification of material type and its surface properties using radial basis networks *IEEE Sens. J.* **8** 1981-91
[14] Mazlum M, Sarpulaku Kh and Savabih H R 2012 The Use of Neural Networks to Optimize the Content of Graphite in Periclase-Graphite Refractories *Novye ogneupory* 41-6
[15] Styrcz A, Mrozek J and Mazur G 2011 A neural-network controlled dynamic evolutionary scheme for global molecular geometry optimization *Int J. Appl. Math. and Comput. Sci.* **21** 559-66
[16] Gordeev L S, Ivanov V A and Stolyarov Yu Yu 1998 Algorithms of Neural Network Modeling of Chemical-Technological Processes *Software Products and Systems* 25-9
[17] Pavlov K F, Romankov P G and Noskov A A 1987 *Examples and Objectives for the Course of Processes and Devices of Chemical Technology,* ed Kurochkina M I and Kuznetsova U K (Leningrad: Chimiya)