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Modeling of absorption process using neural networks

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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).

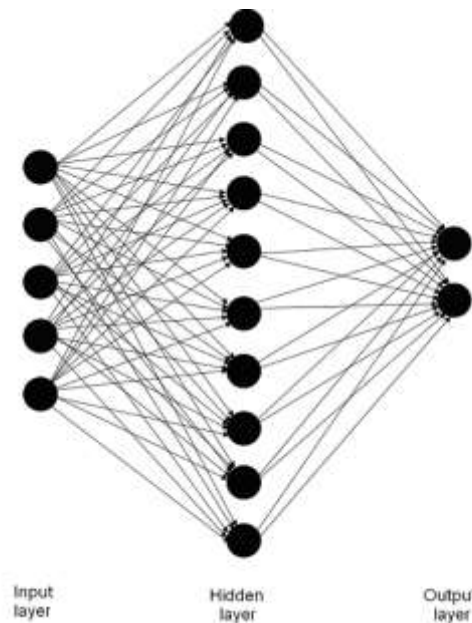


Figure 1. Neural network topology.

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
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Table 4. Output layer W2.

N ^o	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_1
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_r is equal to 3.169. Since $F < F_r$, 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.

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