The basis of an automated design system of the packed absorber using neural networks

O S Kharitonova1,*, I V Vyatkina2, V V Bronskaya3,4, L E Khairullina4, R S Shaikhetdinova5 and N V Kotova1

1Department of Chemical Technology of Petroleum and Gas Processing, Kazan National Research Technological University, 68 Karl Marx Street, Kazan 420015, Russia
2Department of Bilingual Education, Kazan National Research Technological University, 68 Karl Marx Street, Kazan 420015, Russia
3Department of Chemical Process Engineering, Kazan National Research Technological University, 68 Karl Marx Street, Kazan 420015, Russia
4Department of Information Systems, Kazan Federal University, 35 Kremlyovskaya Street, Kazan 420008, Russia
5Department of Technology of Engineering Materials, Kazan National Research Technological University, 68 Karl Marx Street, Kazan 420015, Russia

*E-mail: olga.220499@mail.ru

Abstract. An optimal artificial neural network has been developed for an application to determine the height and diameter of the packed absorber apparatus using neural networks. The obtained results can be used for modeling a wide class of objects of chemical technology with the possibility of formalization of calculation procedures.

1. Introduction
Nowadays there is a growing interest in artificial neural networks. Almost all scientific and technical disciplines conduct research related to the introduction of neural networks to perform applied tasks for simplifying processes or enhancing speed and productivity of these processes.

Due to the massive introduction of artificial neural networks, they are of great interest for various spheres of human life activity, including mechanical engineering.

The growing significance of neural network modeling is due to the growing level of complexity of modern chemical-technological systems and the need of detailed mathematical description [1-3].
2. The main part

Packed columns are widely used in industry devices with continuous phase contact, in which the interphase area is created by bodies of a certain size and a special shape. The packing material that is in the column is placed on the support grilles with holes for liquid and gas. The fluid evenly refluxes the packing material using a distributor and flows in the form of a thin film down the packing material surface. The fluid equilibrium distribution throughout the packing material is usually not achieved due to the wall effect (high loading density of the packing material in the central part of the device). Therefore, the fluid tends to spread out to the column walls from the center. To avoid it, the sections for the packing material which height is not more then 3-4 meters are created in the columns, installing fluid redistributors. As a result, the fluid is redirected from the periphery of the column to its axis.

The technological calculation of the packed absorber is reduced to the determination of the height and the diameter of device, which determine the capital costs in the design of technological equipment. The standard calculation contains the definition of mass transfer coefficients, which generally have a significant deviation from the experimental values due to the inaccuracy of measurements, the presence of impurities, the imperfection of the standard calculation algorithm etc [4-8].

First of all, mol per cent are converted into relative mass concentrations:

$$\bar{Y} = \frac{y_{MA}}{(100 - y)M_B}$$  \hspace{1cm} (1)

where $M_A$ is the absorber molar mass, $M_B$ the inert gas molar mass.

Then we find the consumption of the target component transferred from one phase to another:

$$M = G(\bar{Y}_b - \bar{Y}_f)$$  \hspace{1cm} (2)

using the inert gas flow formula

$$G = \nu \rho$$  \hspace{1cm} (3)

After it is necessary to find the phase-equilibrium constant

$$m = \frac{EM_A}{P_M B}$$  \hspace{1cm} (4)

where $E$ is Henry coefficient. Henry coefficient is represented as table values in the literature. We approximate the available values and get the formula $E = 24289*10^2 + 3*10^5 * r + 7 * 10^7$.

Knowing the value of the phase-equilibrium constant you can find the minimum absorbent consumption:

$$L_{min} = \frac{Mm}{Y_b}$$  \hspace{1cm} (5)

after which the actual consumption is found:

$$L = 1.5L_{min}$$  \hspace{1cm} (6)

Then you need to find the gas velocity. The gas velocity $\omega$ is found in the following way. At first we calculate the fictitious gas velocity $\omega_3$ at the flooding point according to the equation:

$$\lg \left( \frac{\omega_3^2 \sigma \rho_3 \mu_{0.16}}{g V_{fr} \rho_l} \right) = A - 1.75 \left( \frac{L}{G} \right)^{0.25} \left( \frac{\rho_g}{\rho_l} \right)^{0.125}$$  \hspace{1cm} (7)

where $\sigma$ — specific surface of the nozzle, $m^2/m^3$, $g$ — gravitational acceleration, $m/s^2$; $V_{fr}$ — free space of nozzle, $m^3/m^3$; $\rho_l$ and $\rho_g$ — gas and liquid density, $kg/m^3$, $\mu_l$ — dynamic viscosity coefficient of liquid, $mPa*s$; $A$ — coefficient depending on the type of nozzle (in this case -0.073).
Then we determine the operating the gas velocity $\omega$:

$$\omega = 0.8 \omega_j$$

(8)

After it is required to calculate the diffusion coefficient for the gas phase:

$$D_g = \frac{4.3 \times 10^{-7} T^{3/2}}{P(v_{A1}^3 + v_{B1}^3)^3} \sqrt{\frac{1}{M_A} + \frac{1}{M_B}}$$

(9)

where $T$ — temperature, $K$, $M_A$ and $M_B$ — molal masses of gases A and B, $v_A$ and $v_B$ — molal volumes of gases A and B defined as the sum of atomic volumes of the elements that go to make up the gas.

It's also required to calculate the diffusion coefficient for the gas phase:

$$D_l = \frac{1 \times 10^{-6}}{A B \sqrt{\mu (v_{A1}^3 + v_{B1}^3)^2}} \sqrt{\frac{1}{M_A} + \frac{1}{M_B}}$$

(10)

where $\mu$ — dynamic viscosity coefficient of liquid, $\text{mPa s}$, $M_A$ and $M_B$ — molal masses of dissolved matter and solvent; $v_A$ and $v_B$ — molal volumes of dissolved matter and solvent; A and B — coefficients depending on the properties of the dissolved matter and solvent (in this case $A = 1$, $B = 4.7$).

Mass transfer coefficient in the gas phase $\beta_g$ is found according to the equation

$$Nu_g = 0.407 \text{Re}_g^{0.655} (\text{Pr}_g)^{0.33}$$

(11)

Here $Nu_g = \frac{\beta_g d_e}{D_g}$ is the Nusselt number for the gas phase. Therefore $\beta_g$ is equal to:

$$\beta_g = 0.407 \left( \frac{D_g}{d_e} \right) \text{Re}_g^{0.655} (\text{Pr}_g)^{0.33}$$

(12)

where $\text{Re}_g = \frac{4 \omega \rho}{\sigma \mu_g}$ — Reynolds number for the gas phase in the nozzle; $\text{Pr}_g = \frac{\mu_g}{\rho_g D_g}$ — Prandtl number for the gas phase; $\mu_g$ — gas viscosity, $\text{Pa s}$; $d_e$ — equivalent diameter of the nozzle, m.

Mass transfer coefficient in the gas phase $\beta_l$ is found according to the equation

$$Nu_l = 0.0021 \text{Re}_l^{0.75} (\text{Pr}_l)^{0.5}$$

(13)

where $Nu_l = \frac{\beta_l \delta_{red}}{D_l}$ is the Nusselt number for the liquid phase. Consequently,

$$\beta_l = 0.0021 \left( \frac{D_l}{\delta_{red}} \right) \text{Re}_l^{0.75} (\text{Pr}_l)^{0.5}$$

(14)

where $\text{Re}_l = \frac{4L}{\sigma \varphi \mu_l}$ — Reynolds number for liquid phase; $\text{Pr}_l = \frac{\mu_l}{\rho_l D_l}$ — Prandtl number for liquid; $\delta_{red} = \left( \frac{\mu_l^2}{\rho_l g} \right)^{1/3}$ — reduced thickness of liquid film, m; $S = \frac{\pi D^2}{4}$ — cross section of column, $m^2$; $D = \sqrt[4]{\frac{4V}{\pi \varphi}}$ — column diameter, m; $\varphi$ — the moisness coefficient of the nozzle.
The technological calculation of the packed absorber is reduced to the determination of the height and diameter of the device. The standard calculation contains the definition of mass transfer coefficients, which in most cases have a significant deviation from the experimental values due to the inaccuracy of measurements, the presence impurities, the imperfections of the standard calculation algorithm, etc. In connection with it there is a question of determining the mass transfer coefficients using artificial intelligence technologies.

Work on artificial neural networks or just neural networks was initially dictated by the fact that the human brain calculates quite differently than an ordinary computer. In general, a neural network is a machine that is designed to simulate how the brain completes a specific task or function; a network is implemented using electronic components or created a model as software on your computer.

Today sigmoidal function is the most common form of activation function used in the construction of artificial neural networks. It is defined as a strictly increasing function. An example of an activation function of this type is a function called logistic:

$$\phi(\nu) = \frac{1}{1 + \exp(-a\nu)}$$

where $a$ is the slope parameter of the sigmoid function. You can get sigmoidal functions of different slopes changing $a$ (Figure 1). At the limit when the slope parameter approaches infinity, the sigmoidal function becomes just a threshold. While the threshold function takes values of 0 or 1, the sigmoidal function takes a continuous range of values from 0 to 1. Sigmoidal function is differentiable.

![Figure 1. The graph of sigmoidal activation function.](image)

The artificial neural network is a massive parallel distributed processor consisting of simple blocks that has a natural tendency to store empirical knowledge and makes it available for use. The processor reminds the brain because the network receives information from the environment through the educational process and the network has interneurons bonds (synaptic weights) used to store acquired knowledge.[9-12]

3. Results

AForge.NET framework [13] was chosen to implement the artificial neural network of technological calculation of the absorption process. The main applications of the framework are image processing and filters use, artificial neural networks of different architectures, genetic algorithms what is called fuzzy logic, robotics and so on. The framework consists of a set of libraries and samples of applications designed for specific areas of artificial intelligence and computer vision: image and video processing libraries, computer vision libraries, fuzzy computing libraries, neural networks and machine learning libraries.
A multilayer network of direct distribution, which is the most suitable topology for empirical modeling and engineering applications, are used in this paper. A teacher learning method was selected from all network learning methods. The training procedure requires a set of process inputs and outputs. During learning, weights and offsets are iteratively corrected to minimize the target function. The learning algorithm - backpropagation - moves the network parameters in the direction of the negative gradient. The activation function is sigmoidal one with a factor of 2.

The program part was written having formed a general idea of the necessary neural network structure. An artificial neural network in C# language was implemented in Visual Studio 2017 development environment using the AForge.Neuro library. During the work a full-fledged application Windows Forms, which implemented the functions of loading a training selection from a file, setting the necessary training accuracy and entering a vector for obtaining results of neural network operation was created. The application interface is shown in Figure 2. The keyboard input check was implemented — the user has the ability to enter only numbers and separating characters, and full points are automatically replaced with binary points for convenience to record data in the program.

Figure 2. The application interface for working with neural network.

Loading input data from a file and saving data to a file in both parts of the application is implemented. The CSV format was chosen for the files for easy recording and reading. The input vectors are written as “\(V_0; y_n; y_k; t; P\)”. In order to select the structure, errors for each mass transfer coefficients were calculated. The results obtained during the operation of the neural network and obtained by the experiment were compared.

4. Conclusion
Errors of each mass transfer coefficient were calculated to select the architecture. The results obtained during the operation of the neural network and obtained by the experience were compared. The best architecture is the 5-10-2 one based on table 1.
The results of the artificial neural network work showed that the accuracy of determining the height and diameter of the absorber in comparison with theoretical calculations increased at average by 15-20%. The result of the work is an application to determine the height and diameter of the packed absorber device using neural networks.

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

| Architecture | Error $\beta_g$ | Error $\beta_l$ |
|--------------|----------------|----------------|
| 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^{-5} | 8,31043*10^{-7} |
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