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Том 1
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Development of Artificial Neural Networks to Simulate the Process of Dichloroethane Dehydration in the Statistica Software Program

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Abstract – **This paper discusses the application of artificial neural networks for simulation of technological processes. Stages of neural networks designing and training in the Statistica software package as exemplified in the source data of the technological process of dichloroethane dehydration were considered. After training the neural network this program allows to build histograms, scatter grams, graphical representation of the teaching selection on the three-dimensional surface, graphical representation of the training sample on the coordinate plane, etc. These charts help the user clearly see the process of neural network training and evaluate its effectiveness.**

Index Terms – **Neural network, raw material consumption, temperature in the bottom of column; moisture content of dichloroethane, Statistica software program.**

I. INTRODUCTION

USE OF the artificial neural networks is one of the most fast-growing and upcoming trends of the IT-technologies development in the modern world.

Neural network is a system of interacting "neurons". "Neuron" in this case is interpreted as an object with the computing process. The most important feature of neural networks is parallel data processing at hardware implementation, which indicates their powerful capabilities and enormous potential. At the high level of connectivity, parallel data processing provides a means of the information-processing speed-up. Neural networks are effective in such areas as simulation, optimization, prediction, control, speech recognition and so on [1-5].

II. BUILDING OF NEURAL NETWORKS BY THE EXAMPLE OF TECHNOLOGICAL PROCESS OF DICHLOROETHANE DEHYDRATION

Let us develop creating and training of the neural network by the example of the process of the 1,2-dichloroethane dehydration.

Dichloroethane is an intermediate product in the production of vinyl chloride from ethylene and chlorine by liquid-phase chlorination of ethylene in the presence of chlorides of copper, iron or antimony as catalysts.

Heated wet raw dichloroethane is fed into the dehydration column, which is heated by the heat exchangers. Bottom product of the column passes through the filters and is pumped to the stage of distillation of vinyl chloride. Vaporization from the dichloroethane dehydration columns are removed and devaporated. Then the separator detaches dichloroethane, which is sent as phlegm back into the column, and the separated exhaust gases are sent to combustion.

The raw material for dehydration of dichloroethane is raw dichloroethane containing inert gases, low-boiling products, water and impurities. The product of dichloroethane dehydration is purified from impurities, inert gases and low-boiling products 1,2-dichloroethane with mass fraction of water maximum 0.001%.

When carrying out the technological process of dehydration of ethylene dichloride at production site during one month there were obtained a collection of actual experimental data. For multi-objective optimization of the process we selected two main input parameters having significant impact on this process: temperature in bottom of the column and flow rate of the supplied raw materials. Moisture content of dichloroethane serves as the output parameter.

III. PROBLEM DEFINITION

In the present times receiving a dichloroethane of the premium is difficult since it is necessary to control a set of parameters. Moisture content in this process is the key parameter, because the grade of the final product depends on moisture content value. It should not exceed 0.005% for the highest grade (Russian Classification of Production 24 1222 0120), and 0.05% for the first grade (Russian Classification of Production 24 1222 0130) and 0.12% for class II (Russian Classification of Production 24 1222 0140).

IV. CREATION OF THE TABLE WITH BENCHMARK DATA IN THE STATISTICA PROGRAM

After selection of the basic parameters there was prepared a table with the benchmark data for training of the neural network in Statistica software program.

In order to create a table with benchmark data, it is necessary to perform the following steps:

Run the Statistica software program. On the main panel of the program, select ***New*** tab. Choose ***Spreadsheet*** tab in the popup window. Within the ***Spreadsheet*** tab input digit 3 in the field of ***Number of variables***, digit 50 in the ***Number of cases*** field, select ***Double*** in the field of ***Default data type***.

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The selected location is ***As a stand-alone window***. Image format is common (Display format – general). Similarly the other fields were set and OK button was clicked. The program created an empty table with three columns ***Var1, Var2, Var3*** and 50 rows.

After creation of the table, benchmark data were filled in. Also the cell ***Var1*** was selected by double-clicking to change the name and properties of the variable. After that window for editing of the settings of the variable cell ***Var1*** opened. The selected font was Arial, size 10. Indication in the column ***Name Var1*** was renamed for x, measurement scale was transformed in automatic one (measurement type – auto) and also a checkmark was put next to the inscription ***Function guide***. The display format was left to be general. Similar changes were made for the other two variables.

The variables x and y are understood as the input parameters: x is feed rate of raw material, m^3/h; y is the temperature in bottom of the column, °C. The output parameter F is the moisture content of dichloroethane, %. The completed table is shown in the Figure 1. The resulting table with data was saved in file with STA extension.

Data: Spreadsheet1* (3v by 90c)

	1 x	2 y	3 F
1	40	99	0,002323
2	30	32	0,004039
3	38	120	0,001853
4	31	145	0,003185
5	37	92	0,001197
6	34	58	0,001602
7	36	34	0,002718
8	41	133	0,003713
9	41	122	0,003323
10	28	65	0,00383
11	33	82	0,001223
12	37	137	0,002209

Fig. 1. Completed table of benchmark data.

V. Creation of Neural Networks, Training and Testing

After creation and population of the table with data, neural networks were trained and tested in the ***Statistica*** software program.

In the menu bar there was selected the tab of ***Data Mining***. In the toolbar in ***Learning*** item, we selected ***Neural Networks***. Then the window for creating the neural network opened. In the ***New analysis*** field there was selected the analysis type from the given list to create a new analysis ***Regression*** and ***OK*** was pressed.

Then a new window opened to configure the neural network. We selected ***Quick*** tab, marked ***ANC (Automated network search)*** in ***the Strategy for creating predictive models*** field, then pressed ***Variables*** key. After that window appeared where we could choose the variables to be analysed.

Next, we selected variables to build the neural network. In the first window we indicated 3 – F, in the second 1 – x and 2– y. Digit 3 automatically appeared below in the graph of ***Continuous targets*** and 1-2 appeared in the ***continuous inputs*** graph. Next to the ***Show appropriate variables only*** inscription, we removed the checkmark and clicked OK.

After the selection of variables, in the settings window of neural networks, it was observed that the selected values appeared in the ***Variables*** field.

After selection of ***Sampling (CNNN and ANS)*** we input digit 70 in ***Train (%)*** field, digit 15 in Validation (%), digit 15 in ***Test (%)*** field and digit 1000 in ***a Seed of sampling*** item. In the group ***Sampling method*** there were marked ***Random sampling***. After termination up of the neural network setting we pressed ***OK***. In the new window of the parameters group ***Network types*** we put a check mark next to ***MLP*** inscription (multilayer perceptron).

It is possible to determine the required number of neurons in the hidden layers of perceptron by a formula representing a consequence of the theorems of Arnold–Kolmogorov–Hecht-Nielsen:

$$\frac{N_y Q}{1+\log_2(Q)} \le N_w \le N_y\left(\frac{Q}{N_x}+1\right)(N_x+N_y+1)+N_y,$$

$$\frac{1\cdot 35}{1+\log_2(35)} \le N_w \le 1\cdot\left(\frac{35}{2}+1\right)\cdot(2+1+1)+1,$$

$$6 \le N_w \le 75, \quad (1)$$

where N_y is the dimension of the output signal ($N_y = 1$);
N_w is the required number of synaptic connections;
N_x is the dimension of the input signal ($N_x = 2$);
Q is the number of elements of the set of training examples:

$$Q = \frac{50\cdot 70\%}{100\%} = 35.$$

After estimation with the help of this formula the required number of synaptic connections Nw, it is possible to calculate the required number of neurons in the hidden layers. For example, the number of neurons in the hidden layers of two-layer perceptron will be:

$$N = \frac{N_w}{N_x + N_y}. \quad (2)$$

The minimum number of neurons is equal to:

$$N = \frac{6}{2+1} = 2.$$

The maximum number of neurons is equal to:

$$N = \frac{75}{2+1} = 25.$$

Since the range of variation in the number of neurons, offered by default by the ***Statistica*** software, is within the tolerance interval calculated by the formula of Arnold–Kolmogorov–Hecht-Nielsen, we left the interval to be unchanged.

We input digit 3 in the ***Min. hidden units*** field, and digit 9 in the ***Max. hidden units*** field. We entered the following in the group ***Train/Retain networks***: digit 20 in the ***Networks to train*** field, digit 5 in the ***Networks to retain*** item and pressed ***Train*** key. Window for training of the neural networks is presented in the Figure 2.

The results of neural networks training are shown in figure 3. This window contains 5 neural networks with the extremely small values of standard errors for control and test samples.

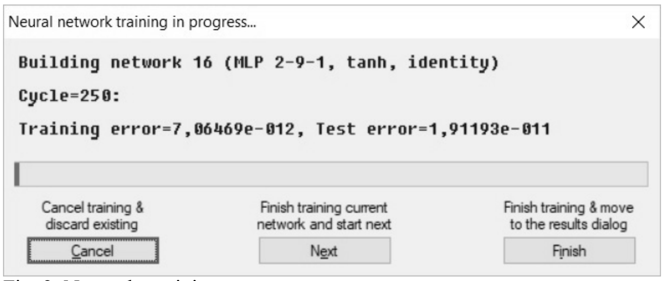

Fig. 2. Networks training.

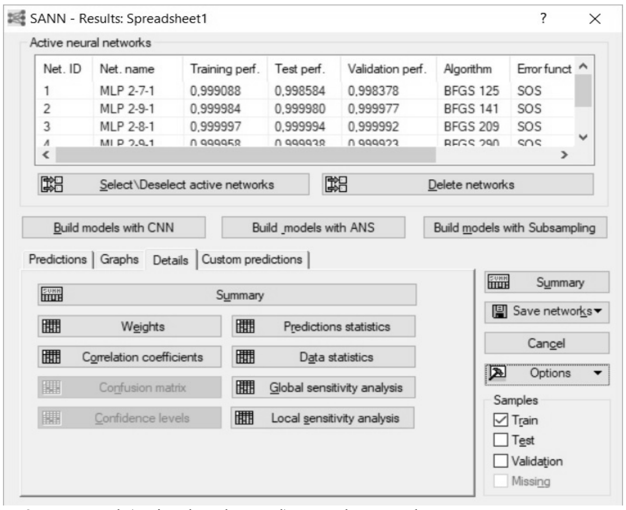

Fig. 3. Prepared (trained and tested) neural networks.

Using neural network trained on the benchmark data, we can construct graphs such as the histograms, scattergrams, graphical representation of the teaching selection on the three-dimensional surface and graphical representation of the training sample on the coordinate plane.

The chart (Fig. 4) presents a graphical representation of the training sample on the coordinate plane where the x-axis is the target (initial) value of F and y-axis is the output value of F obtained by the neural network.

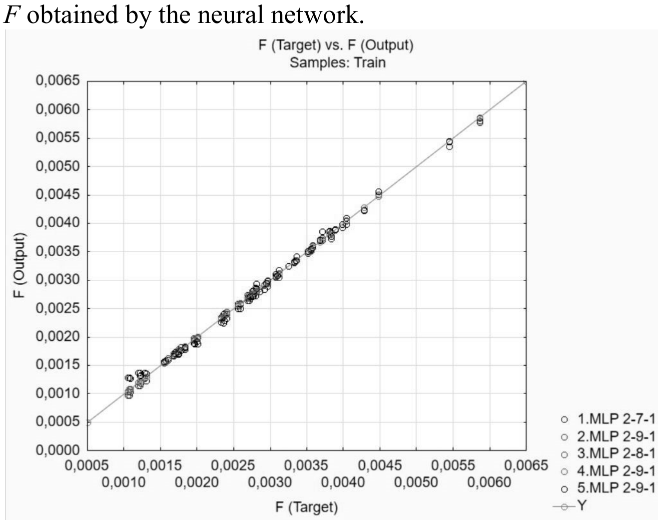

Fig. 4. Scattergram for the training set of the 5 trained neural networks.

During the analysis of the scattergram it is possible to make conclusion about the adequacy of calculation results for all the 5 neural networks. Insignificant deviations are observed only near the borders of the interval of possible values of the target variable.

VI. CONCLUSION

This scientific paper demonstrates preparation of the table with the benchmark data of the technological process of obtaining dichloroethane in the Stastistica software program. With the use of the data obtained there were trained 5 neural networks with the least mean square error. Also, the scattergram was constructed according to the obtained neural network. Due to this scattergram, we can see that the neural networks were trained appropriately in accordance with manufacturing process.

Application of neural networks is the promising direction, which allows in conditions of shortage or complete lack of information on the mathematical regularities, mechanism and kinetics of the simulated process, possessing only data containing numerical values of the main parameters of the process during a certain time period, to build a model which can subsequently be used for optimization, prediction, etc.

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