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MODELING THE WATER ABSORPTION RATE OF WOOD IMPREGNATED WITH SILICONE-BASED CHEMICALS USING AN ARTIFICIAL NEURAL NETWORK

In this study, the water absorption rate of wood impregnated with silicone-based chemicals was predicted by an artificial neural network (ANN). For this purpose, spruce (Picea orientalis L.) and beech (Fagus orientalis L.) wood samples impregnated with five commercial silicone-based chemicals were tested. Wood specimens were impregnated with these chemicals in concentrations of 10% and 50%, and the water absorption rates of samples at different times (2, 4, 8, 24, 48, 72, 168 and 336 hours) were calculated. These results were then modeled by an ANN. Wood species, silicone-based chemical, concentration and time in water were used as the input variables, and water absorption rate as the output variable. The results show that an ANN can be used successfully for predicting the water absorption rate of wood impregnated with silicone-based chemicals.

Keywords: Artificial neural networks, beech, modeling, silicone-based chemicals, spruce, water absorption

Introduction

Wood is one of the most valuable raw materials obtained from renewable sources worldwide, as well as being a unique biopolymer. Wood has numerous advantages over other alternative materials, including high resistance to weight and suitability for use on quite an extensive scale [Tsoumis 1991]. However, like all materials, wood also has disadvantageous properties. Firstly, it is always at risk from pests such as insects and fungi, and can be destroyed by strong acids and bases. Most importantly, it is not stable in form and dimension, because it must balance its moisture content depending on the humidity of its environment [Nicholas 1982]. Water-repellent materials reduce the hygroscopicity of wood; hence they can protect the wood against biotic factors by reducing the amount of

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moisture, which is needed for the growth of fungi and microorganisms [Williams and Feist 1999]. Combinations of water-repellent materials and fungicides (i.e. water-repellent preservatives) are commonly used in wood preservation. In this way, products with dimensional stability and resistance to biological organisms can be obtained [Archer and Cui 1997].

Many studies have been carried out concerning impregnation with silicone, which is regarded as an environmentally friendly chemical because it is not biologically reactive. In a previous study, pine specimens were first modified with maleic anhydride, then reacted with glycidyl ether. The product was finally treated with silicone, and a highly hydrophobic material was obtained [Sèbe and Brook 2001]. The reactivity of cellulose with solvent-borne alkyd-based wood coatings supplemented with organosilanes has been the subject of research. In that study, it was reported that organosilane compounds entered into a chemical reaction with cellulose, and that silane groups were retained in the test samples after all extracellular processes. Therefore, the modification and impregnation processes carried out with the silane groups protected the wood, especially the outer surface, against many abiotic and biotic hazards [Mazela et al. 2010]. In a study by Mai and Militz [2004], wood was modified using various inorganic silicone components, and the strength of the wood was improved. Donath et al. [2006] tested two types of silane groups: monomeric silane compounds (tetralkoxylene, acyl-trialkoxylene) and multifunctional oligomeric silane compounds. They reported that the water absorption of the samples with monomeric silane compounds decreased significantly, but there was no significant change in the case of oligomeric silane compounds. Rosenthal and Bues [2010] used silicone impregnation, considered ecologically friendly, to increase the dimensional stability of pine wood and make it more resistant to fire. Gascón-Garrido et al. [2017] impregnated Scotch pine sapwood in two steps; (1) vacuum-pressure impregnation with amino-siloxane emulsion, and (2) deposition of copper micro-particles on the wood surface using plasma. They reported that the two-step treatment imparted high blue stain resistance to the wood. As scientific studies such as these have shown, the importance of silicone compounds in wood preservation continues to be acknowledged.

In recent years, artificial neural networks (ANNs) have been used in many disciplines, including medicine [Khan et al. 2001; Londhe 2017], engineering [Tiryaki et al. 2016; Gurgen et al. 2018] and the social sciences [Kristjanpoller and Minutolo 2015; Skiba et al. 2017]. ANNs have begun to be applied by scientists in the field of forestry; for example, to simulate long-term effects of varying tree retention on wood production, dead wood and carbon stock changes [Santaniello et al. 2017], to model and optimize a supercritical wood impregnation process [Fernandes et al. 2012], and to predict the compression strength of heat-treated woods [Tiryaki and Aydın 2014]. However, there has been no study to date involving modeling the water absorption rates of wood treated with water-repellent chemicals. Thus, the aim of this study is to model the water absorption rates of wood treated with silicone-based compounds.

Materials and methods

Material

Beech (*Fagus orientalis* L.) and spruce (*Picea orientalis* L.) wood was used in this study. These tree species were chosen taking into account the characteristics of the growing environment, such as direction, slope, diameter, elevation and frequency of the trees, from the Eastern Karadeniz Region Maçka Forestry Office (40°46'10.7"N, 39°39'04.2"E), where they have a natural distribution. To obtain the wood samples used in this study, trees were cut to lengths of 2-4 m and turned into lumber. The cutting process was carried out in accordance with TS 2470 [1976]. Knot-free sapwood samples were used for experimental studies. The resulting parts were left to dry naturally under open air conditions, and after reaching the fiber saturation point they were cut to dimensions according to the standards of the experiment using thickness planning and saw machines. The specific gravity of 20 control samples 2 × 2 × 3 cm in size was determined according to TS 2472 [1976]. Test and control samples were dried at 103 ±2°C in a drying cabinet until they reached constant weight. The specific gravity of the samples was calculated using the following equation:

$$\delta_o = \frac{Mo}{Vo} \left(\frac{\mathrm{g}}{\mathrm{cm}^3}\right) \tag{1}$$

where δ_o is oven dried specific gravity (g/cm^3), *Mo* is oven dried weight (g), and *Vo* is oven dried volume (cm^3).

Silicone-based compounds

The following silicone-based compounds were selected: Dow Corning (R) 1-6184 (Water Repellent), Dow Corning (R) Z-6341 Silane, Dow Corning (R) 2-9034 EU Emulsion, Dow Corning (R) IE 6683 and Dow Corning (R) Z-70. These silicones were in liquid form and obtained from Dow Corning Chemicals (Belgium).

Sample preparation

Samples were prepared in accordance with TS-2470 [1976]. The wood was cut parallel to the grain directions and sawn into specimens measuring 30 (tangential) × 30 (radial) × 15 (longitudinal) mm. All specimens were conditioned at 20 ±2°C and 65 ±3% relative humidity in a conditioning cabinet until their weights became stable. Five separate silicone compounds were prepared with water at two different concentrations, 10% and 50% (volume/ volume).

Wood impregnation

Test specimens were impregnated with the five different silicone compounds at two concentrations. The impregnation of the wood samples was carried out in a laboratory-type impregnation system using the full cell method. Impregnated test specimens were placed in the impregnation vessel and a vacuum of 600 mm/Hg was applied for 30 minutes, followed by a high pressure of 5 bar for 30 minutes. Treated samples were removed from the treatment solution, lightly wiped to remove solution from the wood surface, and weighed to an accuracy of 0.01 g to determine retention values.

Weight percentage gain of wood samples after impregnation

Weight percentage gain values (%) of the samples were calculated by the following equation:

$$\text{Weight percentage gain}\,(\%) = \frac{Mi - Mo}{Mo} \cdot 100 \tag{2}$$

where Mi is the weight of the wood sample after impregnation (g) and Mo is the weight of the sample before impregnation (g).

Water absorption rate

For the calculation of water absorption rate values, it was noted that the samples contain full tangential and full radial directions. The impregnated specimens were dried to constant weight at 103 ±2°C, and the full dry weight and dimensions were determined. They were then left in water, held down with weights placed on top.

Water absorption rates of test and control samples were measured after 2, 4, 8, 24, 48, 72, 168 and 336 hours. In each case, 10 measurements were made and averaged. At the end of each period, water was removed from the surface of the samples and measurements were made at the same sensitivity as before. The water absorption rate was calculated according to following equation:

$$\text{Water Absorption Rate}\,(\%) = \frac{100 \cdot Mi - Mo}{Mo} \tag{3}$$

where Mo is the oven dry mass (g) prior to the test, and Mi is the mass of the sample removed from the water after each period (g).

Statistical analysis

The data were recorded as means ± standard deviation and analyzed using Statistical Package for Social Sciences (SPSS version 13.0). For analysis of the water uptake rate, repeated measures analysis was performed in multivariate analysis and mean values were compared with Duncan homogeneity groups if the effect was significant. The performance of the artificial neural network model was compared with the regression model technique, which is one of the classical methods.

Artificial neural network

Artificial intelligence techniques such as expert systems, artificial neural networks and fuzzy logic have received growing interest in many disciplines. The ANN, inspired by the human brain, is an important tool in classification, prediction, optimization and pattern recognition. The multilayer feed forward neural network is the most commonly used in many engineering modeling scenarios. A typical multilayer network is shown in figure 1.

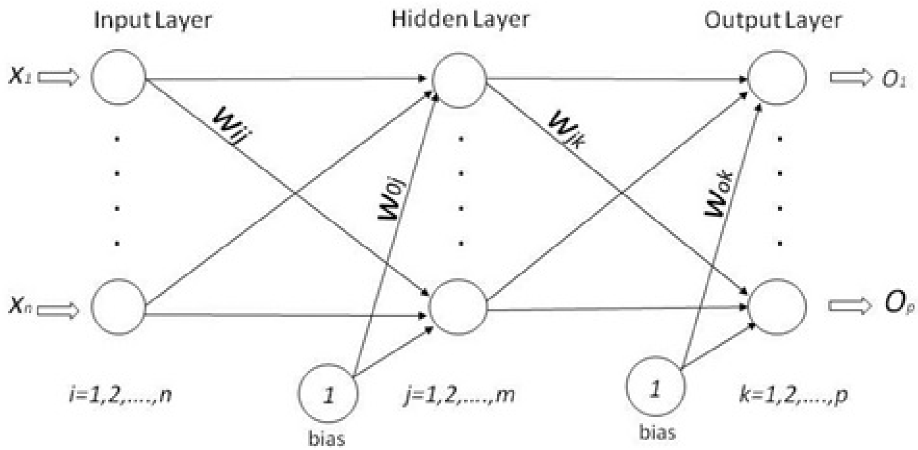

Fig. 1. A typical multilayer neural network

The ANN has an input layer, an output layer and one or more hidden layers linking them [Haykin 1994]. There is no specific rule for the number of neurons in the hidden layer. The most suitable number of neurons with the least error value is determined by the user by trying different numbers of neurons. This selection should be made with care. If excessive neurons are used, the structure of the network can become complicated and the ANN network will be over-fitted [Ozsahin 2013; Tiryaki et al. 2014]. Output values are determined by the following equation:

$$output_k = f_2\left(w_{0k} + \sum_{j=1}^{m} w_{jk}\left[f_1\left(w_{0j} + \sum_{i=1}^{n} x_i w_{ij}\right)\right]\right) \quad (4)$$

where x_i is the value of the input, n is the number of input neurons, w_{ij} is the weight between the input neurons and the hidden neurons, w_{0j} is the bias weight of the hidden layer, w_{jk} is the weight between the hidden and the output neurons, *m* is the number of neurons of the hidden layer, *p* is the number of neurons of the output layer, w_{0k} is the bias weight of the output layer, and f_1 and f_2 are activation functions in the hidden layer and the output layer respectively. The logistic sigmoid and linear functions are used as the activation functions in the hidden and output layer; mathematical definitions are expressed in the following equations (5) and (6):

$$f_1 = \frac{1}{1+e^{-x}} \quad (5)$$

$$f_2 = x \quad (6)$$

The most popular learning algorithms are back-propagation and its variants. The main purpose of all algorithms is to minimize the global error at the ANN training stage. In general, the mean square error (MSE) is used, given by equation (7):

$$MSE = \frac{1}{n}\sum_{i=1}^{n}\left(t_i - o_i\right)^2 \quad (7)$$

where *t* is the target value, *o* is the output, and *n* is the number of samples.

To construct the ANN model, the existing data are divided into three sets for training, validation and testing. The training data set is used only for network training. Learning in the ANN is carried out by updating the weights among the nodes. The validation data set is used to prevent memorization of the network. If validation is not used, the ANN network may tend to memorize instead of learning. Finally, the performance of the trained ANN is evaluated using the test data set, which was not used during the training phase.

Application of an artificial neural network

The aim of this study was to develop an artificial neural network model to predict water absorption rates for spruce and beech wood samples. Wood species, chemical type, concentration rate and time in water were used as the input parameters, and water absorption rate as the output parameter. Figure 2 illustrates the structure of the neural network model for the present study.

Two different wood species, five chemical types, two concentration rates and eight times in water were used in the study, giving a total of 160 samples. Among the data, 112 random data points (70% of the total) were used as the training set, 24 data points (15% of the total) were used as the validation set, and the remaining 24 data points (15% of the total) were used for performance testing. In this study, the Levenberg–Marquardt (LM) algorithm was applied for the single hidden layer. The ANN was trained and tested using MATLAB software. The performance goal for training was set to 10^{-2}. The MSE was determined as the network performance function. The architecture of the ANN model is summarized in table 1.

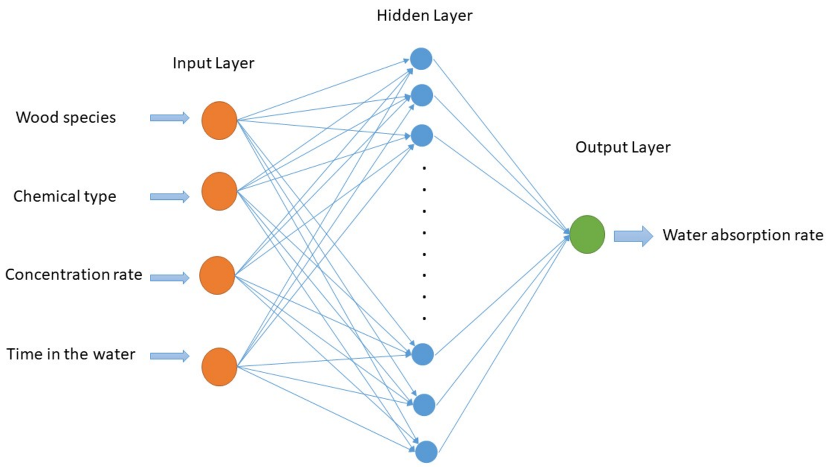

Fig. 2. The structure of the neural network model

Table 1. Architecture of the ANN model

Parameters	Value
Training algorithm	Levenberg–Marquardt (trainlm)
Performance function	Mean square error (mse)
Hidden layer activation function	Logistic sigmoid (logsig)
Output layer activation	Linear transfer function (purelin)
Number of hidden layers	1
Input layer nodes	4
Hidden layer nodes	1.05.2020
Output layer nodes	1
Maximum validation error iterations	50

The prediction performances of the trained ANN and the regression model were determined using statistical expressions for MAPE, RMSE and coefficient of determination (R^2). These values are expressed by the following equations (8), (9) and (10):

$$MAPE = \frac{1}{n} \sum \left| \frac{t_i - o_i}{t_i} \right| \cdot 100 \tag{8}$$

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (t_i - o_i)^2} \tag{9}$$

$$R^2 = 1 - \frac{\sum_{i=1}^{n} \left(t_i - o_i\right)^2}{\sum_{i=1}^{n} \left(o_i - \acute{o}\right)^2} \tag{10}$$

where t is the target value, o is the output, $\acute{o}$ is the mean of the output, and n is the number of samples.

Results and discussion

Oven-dried specific gravity was determined at 0.44 ±0.03 and 0.73 ±0.05 g/cm^3 for spruce and beech wood samples respectively. Average weight percentage gain (X) and standard deviation (S) values of the samples treated with different solutions are summarized in table 2.

Table 2. Average weight percentage gain values of spruce and beech wood samples

Impregnation solution	Concentration (%)	Spruce		Beech	
		X*	S**	X	S
Dow Corning (R) 1-6184	50	14.34	3.87	8.38	0.96
	10	11.86	1.78	7.70	0.37
Dow Corning (R) Z-6341	50	34.44	8.33	25.23	1.87
	10	7.87	2.77	9.11	3.99
Dow Corning (R) 2-9034	50	20.84	4.21	29.96	1.74
	10	6.38	0.70	9.41	3.27
Dow Corning (R) IE-6683	50	23.04	3.56	30.03	9.36
	10	5.75	0.62	20.43	4.67
Dow Corning (R) Z-70	50	36.82	9.83	41.11	9.43
	10	8.85	1.09	15.72	3.68

* Arithmetic mean.
** Standard deviation.

The weight percentage gain values of the spruce wood samples were found to lie between 5.75% and 36.82%. For beech wood samples, values lay between 7.70% and 41.11%. Compared with the other compounds, Z-70 exhibited better performance for both wood species. Z-70 may have formed a better bond and provided more functional components that can be polymerized in the wood structure. It is known that spruce impregnation is difficult. It is also clear from table 2, however, that with both concentrations of 1-6184, and with the higher concentration of Z-6341, weight percentage gains in the spruce wood were higher than in beech wood. As an explanation for this, the high values of weight percentage gain obtained for spruce samples may be related to anatomical characteristics. Pore space may be much greater locally in the spruce samples.

The maximum and minimum water absorption rates of the impregnated wood species are presented in table 3. In this study, the lowest water absorption rate was found in spruce samples impregnated with a 50% concentration of Dow Corning (R) 2-9034 EU, and the highest in spruce samples impregnated with a 10% concentration of Dow Corning (R) 1-6184. For beech samples, the highest and the lowest water absorption rates were obtained respectively for samples impregnated with a 10% concentration of Dow Corning (R) Z-6341 Silane and a 50% concentration of Dow Corning (R) Z-70. Similarly, to our study, in a previous study by Tshabalala and Gangstad [2003], *Pinus taeda* test samples were treated with polysiloxane to prevent washing after impregnation with a mixture of methyltrimethoxysilane and hexadecyltrimethoxylane, and good water repellency was obtained. Terziev et al. [2009] investigated the water--repellent effectiveness and dimensional stability of Scots pine test specimens in laboratory conditions using a mixture of silicon and boron, but did not obtain a positive result. The homogeneity groups of variations are presented in table 4.

Table 3. Water absorption rate of impregnated wood species

Wood species	Water absorption rate (%)	
	Minimum	Maximum
Spruce	10.21	149.26
Beech	1.66	96.68

As seen in table 4, according to the results of multivariate analysis, significant statistical differences were found among the water absorption rates of test samples of both wood species.

Table 4. Homogeneity groups of variations

Variations	Homogeneity groups	
	Spruce	Beech
Dow Corning (R) 1-6184	b	e
Dow Corning (R) Z-6341	b	b
Dow Corning (R) 2-9034	c	e
Dow Corning (R) IE-6683	b	d
Dow Corning (R) Z-70	a	c
Control	a	a

In order to obtain the best output values for the experimental data, different numbers of neurons (5-20) in the hidden layer were tried. Table 5 gives the MAPE and regression (R) values for the complete data set for different hidden neuron numbers. It may be seen from this table that the minimum error was obtained when the number of hidden nodes was chosen as 16. The *MAPE* and R values for 16 hidden neurons in the LM algorithm were found to be 3.823649 and 0.9919 respectively.

Table 5. Performance of different numbers of hidden neurons

Hidden neurons	*MAPE*	R
5	11.91873	0.977478165
6	9.663595	0.988274496
7	8.323227	0.990929839
8	8.766234	0.990229531
9	6.565629	0.991649554
10	6.414529	0.992469643
11	5.297868	0.991813482
12	5.824134	0.992967649
13	5.939906	0.995256415
14	5.812344	0.990624130
15	4.283712	0.978500210
16	3.823649	0.991925763
17	4.894722	0.992028638
18	4.065516	0.990067867
19	4.80966	0.991189689
20	4.465197	0.986641393

Table 6 shows the *MAPE*, *RMSE* and R^2 values of the optimum neural network model and regression model in detail. As is shown in the table, *MAPE*s were obtained as 1.9387, 6.9706, 9.4727 and 3.8236, and *RMSE* values as 0.879, 4.6701, 9.4983 and 4.1647, respectively for the training, validation and test data sets and for all data sets. R^2 values were computed as 0.993, 0.9809, 0.8951 and 0.9839 for the same data sets. Thus, the *MAPE* has an acceptable value, below 10%. Since the R^2 value is very close to 1, it can be stated that the experimental results are in agreement with the ANN model results. *MAPE*, *RMSE* and R^2 values for the regression model were determined at 50.78710, 13.2670 and 0.7595 respectively. All performance values of the regression model were lower than for the ANN model. In a previous study, in which the properties of corrugated base papers were predicted using multiple linear regression and artificial neural networks, it was reported that ANN models gave more accurate results than regression models [Adamopoulos et al. 2016]. Consequently, the results of this study are in agreement with the previous literature.

Table 6. Performance values of ANN and regression model

Data set	*MAPE*	*RMSE*	R^2
Training data	1.938779	0.879	0.993
Validation data	6.970647	4.6701	0.9809
Testing data	9.472713	9.4983	0.8951
All data	3.823649	4.1647	0.9839
Regression model	50.78710	13.2670	0.7595

Figure 3 shows the performance plot of the developed network at the training stage. After the 90th epoch, the validation and test sets exhibited an increasing trend. The training of the network was stopped because there was no reduction during 50 iterations. Hence, the best validation performance was achieved at epoch 90. The mean square error was calculated as 21.8095.

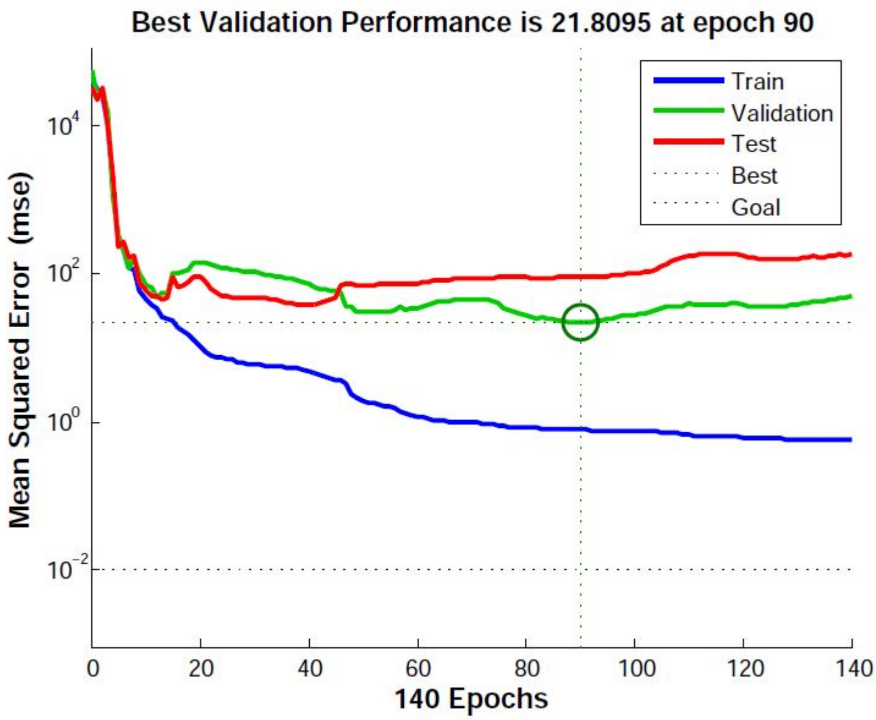

Fig. 3. Performance plot of the developed network

The regression graphic between the estimated ANN values and experimental water absorption rate is shown in figure 4. The correlation coefficients are 0.99966, 0.99043, 0.94609 and 0.99193 respectively for the training, validation and test data sets and for all data sets. These results indicate that the actual values and the predicted values are consistent.

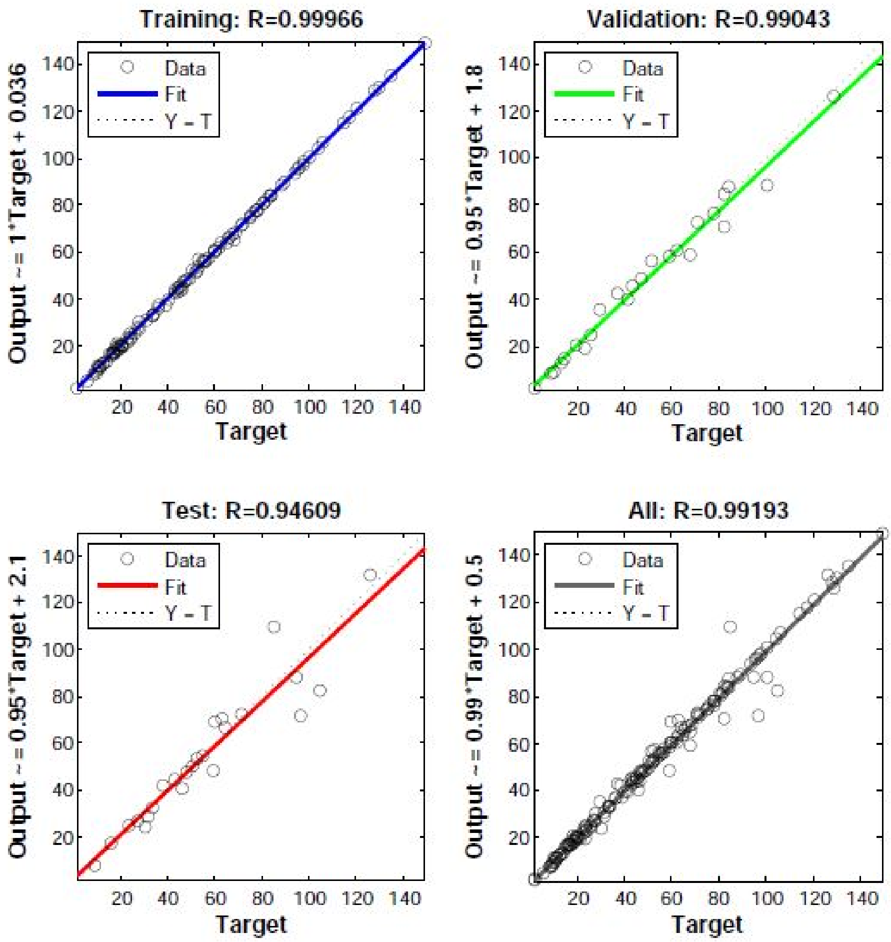

Fig. 4. Regression graphics of the developed network

The error histogram is shown in figure 5. The blue, green, and red bars denote the training data, validation data and testing data respectively. The error value is calculated as the difference between the experimental and the predicted value. The orange line marks the zero error line. It is clear that the largest portion of data coincided with the zero error line. In general, errors are seen to range between –1.067 and –1.391.

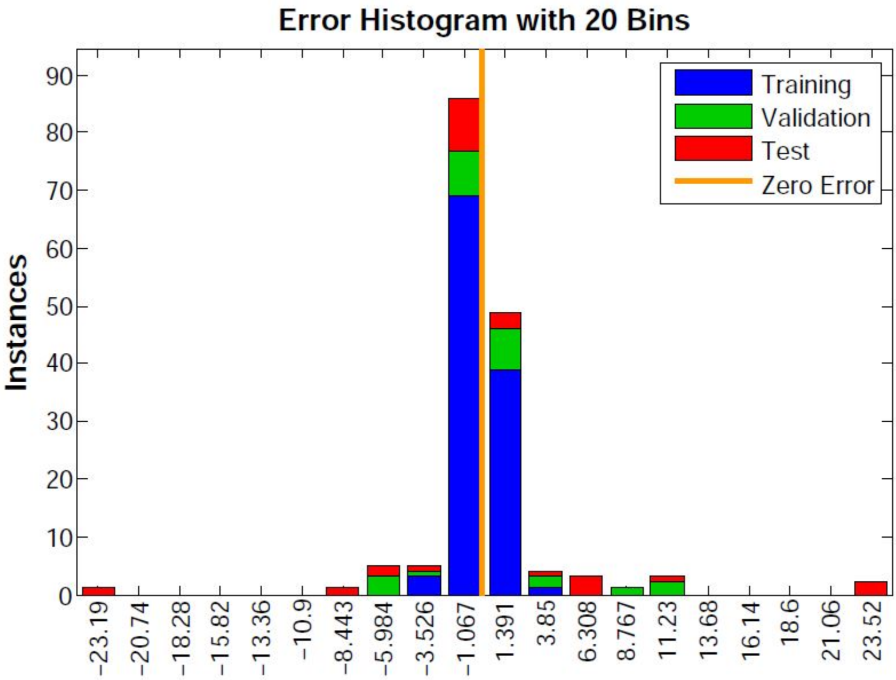

Fig. 5. Error histogram of developed ANN model

Conclusions

An ANN model was constructed to predict the water absorption rate of wood impregnated with different silicone-based compounds. The results demonstrate that the ANN model is a sufficient and successful tool to predict the water absorption rate of wood samples impregnated with such compounds, saving time and costs at the experimental stage. In addition, while ANN applications generally relate to machine processes – for example, they may concern the mechanical properties of wood in the forest engineering industry – this model also demonstrates their applicability in the field of wood protection. The conclusions of this study may be summarized as follows;

- The 4-16-1 neuron configuration was determined as the optimal configuration.
- *MAPE*s were found to be 1.9387, 6.9706, 9.4727 and 3.8236 respectively for the training, validation and test data sets and for all data sets.
- *RMSE* values were found to be 0.879, 4.6701, 9.4983 and 4.1647 respectively for the training, validation and test data sets and for all data sets.

- R^2 values were computed as 0.993, 0.9809, 0.8951 and 0.9839 respectively for the training, validation and test data sets and for all data sets.
- The best validation performance was achieved at epoch 90. The *MSE* was calculated as 21.8095.
- In general, errors are seen to range between –1.067 and –1.391.

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