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# Prediction of Properties of Microwave-Hardened Sandmixes Containing Water-Glass with Use of Neural Networks

**M. Stachowicz*, Ł. Pałyga, K. Granat**
Wroclaw University of Technology, Department of Foundry Engineering, Plastics and Automation, Smoluchowskiego 25, 50-372 Wrocław, Poland
*Corresponding author. E-mail address: mateusz.stachowicz@pwr.edu.pl

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## Abstract

Presented are results of a research on the possibility of using artificial neural networks for forecasting mechanical and technological parameters of moulding sands containing water-glass, hardened in the innovative microwave heating process. Trial predictions were confronted with experimental results of examining sandmixes prepared on the base of high-silica sand, containing various grades of sodium water-glass and additions of a wetting agent. It was found on the grounds of obtained values of tensile strength and permeability that, with use of artificial neural networks, it is possible complex forecasting mechanical and technological properties of these materials after microwave heating and the obtained data will be used in further research works on application of modern analytic methods for designing production technology of high-quality casting cores and moulds.

**Keywords:** Foundry engineering, Artificial neural networks, Loose self-hardening moulding sand, Water-glass, Microwaves

## 1. Introduction

As demonstrated by previous research works, moulding sands containing water-glass can be successfully hardened using microwave energy with frequency 2.45 GHz [1, 2, 3]. Microwave heating of loose self-hardening moulding sands [4], prepared with various kinds of binders, can be an alternative solution for many well-known and applied hardening methods, like the $CO_2$ process, i.e. blowing-through with carbon dioxide at controlled temperature [6], drying with air at elevated temperature or hardening by means of liquid esters. Microwave heating of moulding sands containing hydrated sodium silicate can be the technology complementing the above-mentioned methods of bonding bas grains. However, in order that this eco-friendly and economical [7] technology could be widely applied in practice, it is required more detailed knowledge of microwave heating and complete knowledge of the factors and phenomena decisive for mechanical and technological parameters of the hardened sandmix.

Knowledge about possibly largest number of the factors affecting parameters of a hardened moulding sand can be gained, for example, by standard statistical analysis based on empirical data acquired for a properly numerous population.

In the case of the innovative method of microwave hardening of moulding sands containing water-glass, typical linear and non-linear models describing selected relationships between individual components of the sandmix and the obtained parameters of such mixtures after hardening can deliver only a fragmentary (two- or less often three-dimensional) description of the relationships related to the hardening process [8, 9]. The output function, describing e.g. mechanical strength, results often from the relation between one input constant and one, sometimes two (Fig. 1) [10] variables being qualitative components of the sandmix (e.g. amount of the binder). This approach requires a very large number of experiments. However, so large number of input variables creates a difficulty of their complex analysis and thus prediction of strength of the moulding sand after its microwave hardening is also difficult. Shortage of knowledge on quantity and selection of components of sandmixes causes that implementing this solution in foundry practice, where technology of moulding sands is mainly responsible for quality of manufactured castings, is nowadays a very difficult or even unfeasible task.

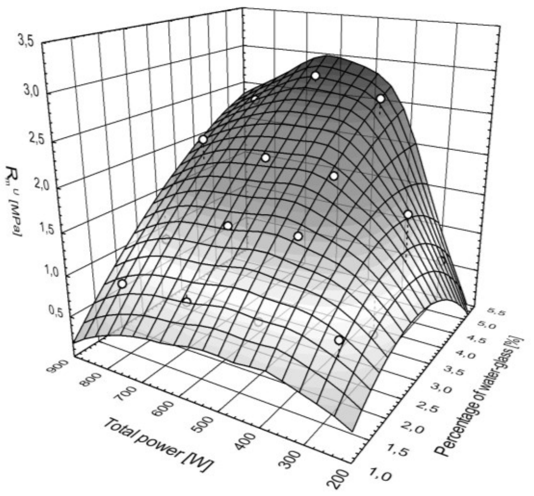


Fig. 1. Effect of fraction of the binder 137 and microwave power on tensile strength of hardened moulding sand

The relationships in moulding sands, containing large numbers of input variables, both quantitative and qualitative, are described in a complex way using artificial neural networks [11-13]. The neural networks are currently the most modern, flexible and sophisticated element of mathematical analysis used for modelling extremely complex functions and relationships. Thanks to the generated models, built using the train function of neural networks on the grounds of the empirically acquired knowledge, it is possible to use them for predicting properties of moulding and core sands based on completely new data with identical structure, but not being real experimental results. In the further text presented are preliminary analyses of applying artificial neural networks for building a model that enables forecasting selected mechanical and technological properties of moulding sands containing water-glass, hardened by microwave heating.

## 2. Purpose of the research

Both strength and permeability of moulding sands are affected by numerous factors. The previous statistical analyses and microscopic observations [14] made it possible to separate those factors, whose influence can be significant from the viewpoint of creating linking bridges between the base grains. They include kind and amount of water-glass and also grade of high-silica sand (main fraction), as well as presence of possible additives. Significance of the above-mentioned factors can be of different importance for the hardening process and requires additional sensitivity analysis.

The constant parameters of the microwave heating process, determined in the previous examinations, like minimum hardening time (Fig. 2) [9], microwave power (Fig. 3) [8] and constant filling of the working chamber, guaranteed full repeatability of parameters of the hardened sandmix. These data served as a basis for further trials of determining, which of the moulding sand components play so much important role that they can be used for developing a model of the microwave hardening process that would ensure complete control of its parameters and results.

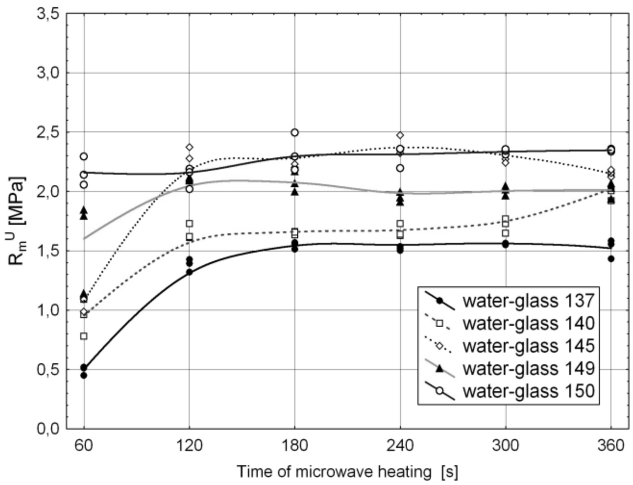


Fig. 2. Effect of microwave heating time and grade of water-glass on tensile strength of hardened moulding sand

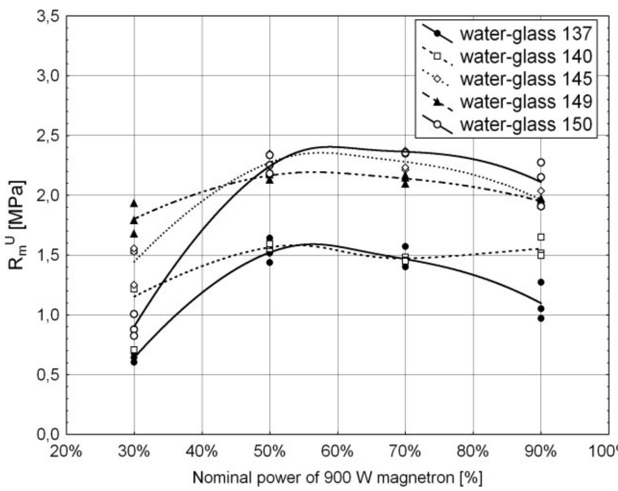


Fig. 3. Effect of microwave power and grade of water-glass on tensile strength of hardened moulding sand

## 3. Methodology of the research

It was found in the preliminary research on building a complex model of microwave hardening that tensile strength $R_m^U$ of a hardened sandmix and its permeability $P^U$ will belong to the group of main output factors serving as selection criteria of the sandmix composition for the given manufacturing process. An attempt was made to build a model using one of the most popular artificial neural networks type MLP (multilayer perceptron). The choice was motivated by nature of the phenomenon and the possibility of training the network in the supervised mode, i.e. with a teacher, in that known are required values of some output data in the built model. Structure of a multilayer perceptron consisting of the input layer, hidden layers and the output layer is shown in Fig. 4. Each neuron of the network calculates weighted average of the supplied inputs, i.e. the so-called weights; the result is converted by means of the transfer function *f* and fed to the output [15]. Such a network with proper number of layers and neurons in these layers can model the relationship with almost any complexity. Selection of proper numbers of hidden layers and neutrons in them was performed in the program Statistica 10.

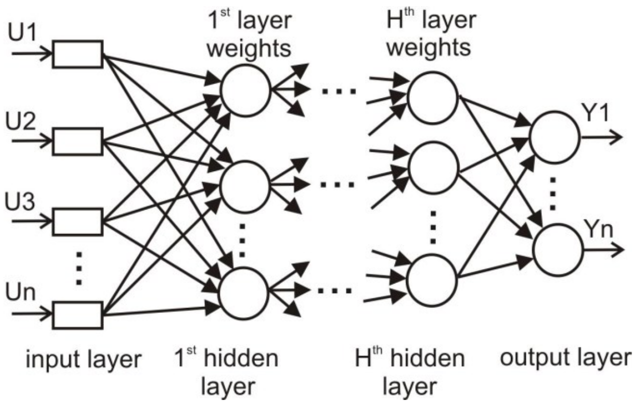


Fig. 4. Example of artificial neural network type MLP

In the research used were 28 combinations of input data 3 tests each, which made in total 84 single measurements of tensile strength and 84 single measurements of permeability taken according to PN-83/H-11073 and PN-83/H-11072.

It was established that the quantitative input in the mathematical model will be:
U1 = amount of binder added to the sand in % by weight.

Due to the given physico-chemical data ranges (Table 1) specified by the manufacturer of the unmodified commercial kinds of water-glass, in the mathematical model it is proposed to averaging these values which will have further function as a qualitative input variables:
U11 = kind of the binder acc. to average molar module, or
U12 = kind of the binder acc. to content of oxides, or
U13 = kind of the binder acc. to average density.
These variables served as a basis for further trials of determining, which of the water-glass details play so much important role that they can be used for developing a model of the microwave hardening process.

Moreover, the qualitative input will be:
U23 = kind of the high-silica moulding sand (Table 2).

Constant values in this model will be:
C1 = hardening time of 240 s [9],
C2 = microwave power of 810 W [8],
C3 = filling of the microwave furnace chamber with the sandmix of 450 g ±50 g,
C4 = content of water as a special wetting additive added to 0.5% at the beginning of the stirring process,
C5 = systematic error of measuring devices,
C6 = ambient temperature of 25 °C ±3 °C
C7 = ambient humidity of 35% ±5%,
C8 = compacting method acc. to PN-83/H-11070.

Dependent outputs in the model, and at the same time indices used for selection of the sandmix components for the given manufacturing technology, will be:
Y1 = tensile strength after microwave hardening $R_m^U$ [MPa],
Y2 = permeability after microwave hardening $P^U$ [$10^{-8}m^2/Pa*s$].

Table 1.
Physico-chemical properties of water-glass contained in the moulding sands with coding of combinations of qualitative variables U11, U12 and U13

| Kind of water-glass: | 137 | 140 | 145 | 149 | 150 |
|---|---|---|---|---|---|
| Molar module $SiO_2/Na_2O$ | 3.2÷3.4 | 2.9÷3.1 | 2.4÷2.6 | 2.8÷3.0 | 1.9÷2.1 |
| Average molar module (U11) | 3.3 | 3.0 | 2.5 | 2.9 | 2.0 |
| Coding of qualitative variable (U11) | 1 | 2 | 4 | 3 | 5 |
| Content of oxides ($SiO_2$+$Na_2O$) % (U12) | 35.0 | 36.0 | 39.0 | 42.5 | 40.0 |
| Coding of qualitative variable (U12) | 1 | 2 | 3 | 5 | 4 |
| Density at 20 °C [g/cm$^3$] | 1.37 ÷1.40 | 1.40 ÷1.43 | 1.45 ÷1.48 | 1.49 ÷1.51 | 1.50 ÷1.53 |
| Average density (U13) | 1.385 | 1.415 | 1.465 | 1.500 | 1.515 |
| Coding of qualitative variable (U13) | 1 | 2 | 3 | 4 | 5 |
| Dynamic viscosity, min. (P) | 1 | 1 | 1 | 7 | 1 |

In the built model were used the data acquired for the sandmixes prepared with high-silica sand, the most popular material for bases of sandmixes containing water-glass. Table 2 includes typical main fractions of high-silica bases acc. to PN-85/H-11001 [16].

Table 2.
Classification of high-silica base acc. to total mesh fractions calculated from three neighbouring sieves with coding of qualitative variable U23

| Kind of sand: | Coding of qualitative variable (U23): | Main fraction [mm]: |
|---|---|---|
| Coarse | 4 | 0.40/0.32/0.20 |
| Medium | 3 | 0.32/0.20/0.16 |
| Fine | 2 | 0.20/0.16/0.10 |
| Very fine | 1 | 0.16/0.10/0.071 |

For the above-described set of data performed was a series of experiments aimed at building toe most favourable model for forecasting mechanical and technological properties of moulding sands containing water-glass, hardened with microwaves.

The starting point, apart from a review of the input and output parameters of the hardening process, were analyses of linear regression models. To build these models were used quantitative data from Table 1, represented by the average value of the compartments of physico-chemical parameters of water glass kinds. It can be found on the grounds of the results of matching to linear models describing influence of such a binder detail (Table 3) that they are random and, in addition not fully matching (Pearson's correlation coefficients) so that they could play the role of valuable models for forecasting mechanical parameters, like tensile strength.

Table 3.
Exemplary results of statistical analysis for linear model developed for various types of water-glass and selected coarse-grained base

| Parameter $R_m^U$ acc. to: | The determined correlation coefficients are consistent with the condition $p < 0.05$. | | | | |
|---|---|---|---|---|---|
| | Standard deviation | r(X,Y) | $r^2$ | t | p |
| U11 | 0.4115 | - 0.8475 | 0.7183 | - 2.7656 | 0.0698 |
| U12 | 0.4115 | 0.8426 | 0.7099 | 2.7096 | 0.0732 |
| U13 | 0.4115 | 0.9484 | 0.8995 | 5.1830 | 0.0139 |

Like the linear regression models, multidimensional analyses are characterised by relatively small accuracy of matching (Table 4) and scatter of residuals does not meet one of the assumptions about their random distribution, i.e. about the so-called point cloud. The possibility of describing the relationship by a polynomial function is shown in Fig. 5 together with the diagram of scatter of residuals with respect to the predicted values.

Table 4.
Matching of multiple analyses for qualitative variables U11, U12 and U13

| Paramete r $R_m^U$ acc. to: | The determined correlation coefficients are consistent with the condition $p < 0.05$. | | | | |
|---|---|---|---|---|---|
| | Standard deviation | r(X,Y) | $r^2$ | t | p |
| U11 | 0.32687 | 0.93803 | 0.87991 | 0.51858 | 0.6055 |
| U12 | 0.35437 | 0.92675 | 0.85887 | 2.02262 | 0.0465 |
| U13 | 0.34127 | 0.93225 | 0.86910 | 1.83100 | 0.0708 |

The performed analyses of linear and multidimensional models clearly directed searching the forecasting model on artificial neural networks. Before starting examinations on these networks, the input data and their corresponding dependent outputs were divided to three sets: training, testing and validation one.

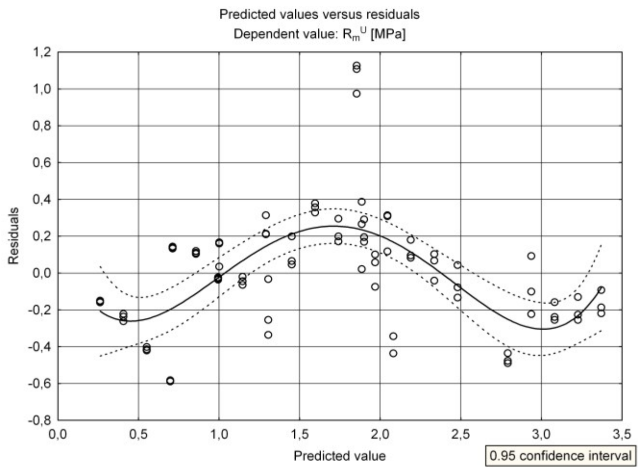


Fig. 5. Scatter of residuals versus predicted values for multidimensional analysis

# 4. Results

The model was built using neural networks type MLP with one hidden layer. Training simulations of the automatically generated networks were repeated three times, reaching the number of 1200 models in each of the considered cases. In these models used were various combinations of the neuron activation functions, like hyperbolic tangent and exponential function for the hidden and output layers.

The hyperbolic tangent as an activation function often acts better than a logistic function, also possible to be applied in the simulation program. This is a S-shaped symmetrical curve with its output values located within -1 to +1. The exponential activation function is a combination of a radial aggregation function and an exponential function with a negative exponent. It defines the neurons modelling the Gauss function centred with respect to the weight vector [15].

Training of the network was performed with the quasi-Newton method type BFGS (Broyden-Fletcher-Goldfarb-Shanno), considered the most effective one among those available in the simulation program [15]. The optimum (final) set of weights of the network was obtained at the moment of minimum root-mean-square error for the validation set. Thus, used was the sum of squares (SOS) method for the deviations between the set value and the network output.

Size of the input layer was determined by the quantitative variable (U1) and the way of coding the qualitative variables (U11 or U12 or U13 and U23) using One-of-N encoding method. This is the basic encoding method, commonly used in the preliminary tests [15], characterized by a large number of neurons in the input layer. During training, one neuron for each possible quantitative value is on while the others are off. Size of the hidden layer was accepted experimentally following the data available in literature [17, 18] and those from own experiments, trying to eliminate the risk of unfavourable effect of overtraining the model, i.e. the phenomenon of excessive matching the network to the training data. Overtraining of the network is most often caused by too large number of neurons in the hidden layer. Adding qualitative variables (U11 to U13 and U23) to the model resulted in the necessity to use additional input neurons. However, it should be noted that the examined models are not the final ones, but are only starting points for further analyses consisting in combining subsequent elements composing the innovative microwaves heating process of core and moulding sands in order to forecast possibly largest number of effects in form of their mechanical and technological parameters after hardening.

On the grounds of the simulations for the variables U1, U11 and U23, determined was structure of the network $MLP_1$: 10-6-2 with 106 cycles of training, with activation of hidden neurons of hyperbolic tangent type and activation in the output layer of exponential type.

On the grounds of the simulations for the variables U1, U12 and U23, determined was structure of the network $MLP_2$: 10-5-2 with 167 cycles of training, with activation of hyperbolic tangent type in the hidden and output layers.

On the grounds of the simulations for the variables U1, U13 and U23, determined was size of the hidden layer in the network $MLP_3$: 10-6-2 with 174 cycles of training, with activation of hyperbolic tangent type in the hidden and output layers.

For the generated artificial neural networks with minimum root-mean-square errors for the validation set, Table 5 includes Pearson's correlation coefficients for the training, testing and validation sets, being measures of their matching to the set of input and output data.

Table 5.
Pearson's correlation coefficients for the generated artificial neural networks MLP

| Net-work: | Output variable $R_m^U$ | | | Output variable $P^U$ | | |
|---|---|---|---|---|---|---|
| | Train-ing | Test | Vali-dation | Train-ing | Test | Vali-dation |
| $MLP_1$ | 0.9966 | 0.9954 | 0.9939 | 0.9933 | 0.9875 | 0.9864 |
| $MLP_2$ | 0.9967 | 0.9953 | 0.9940 | 0.9968 | 0.9946 | 0.9888 |
| $MLP_3$ | 0.9944 | 0.9938 | 0.9908 | 0.9964 | 0.9950 | 0.9902 |

Table 6 includes analyses related to sensitivity of the models to individual quantitative and qualitative input variables suggested in Tables 1 and 2.

Table 6.
Sensitivity analysis for quantitative and qualitative variables in the MLP networks

| **$MLP_1$: 10-6-2**: | U1 | U11 | U12 | U13 | U23 |
|---|---|---|---|---|---|
| Training Error | 14.28 | 8.20 | - | - | 572.87 |
| Training Rank | 2 | 3 | - | - | 1 |
| Error Valid. | 8.05 | 5.12 | - | - | 313.77 |
| Rank Valid. | 2 | 3 | - | - | 1 |
| **$MLP_2$: 10-5-2:** | | | | | |
| Training Error | 35.11 | - | 224.14 | - | 3291.86 |
| Training Rank | 3 | - | 2 | - | 1 |
| Error Valid. | 14.47 | - | 41.78 | - | 1351.68 |
| Rank Valid. | 3 | - | 2 | - | 1 |
| **$MLP_3$: 10-6-2**: | | | | | |
| Training Error | 29.24 | - | - | 64.35 | 148.85 |
| Training Rank | 3 | - | - | 2 | 1 |
| Error Valid. | 15.03 | - | - | 45.73 | 466.77 |
| Rank Valid. | 3 | - | - | 2 | 1 |

It can be seen on the grounds of the data in Table 5 that in all the MLP networks obtained were high values of Pearson's coefficients for both output variables $R_m^U$ and $P^U$ at each stage of training the network: training, testing and validation. The chosen networks are characterised by high level of matching the generated models to the input and output data with relatively short training cycles.

It can be seen on the grounds of the data in Table 6 that, in each of the analysed cases, the process of training the neural networks is most intensively affected by the qualitative variable U23 being a combination of coding a grade of high-silica sand, see Table 2. Therefore, it can be assumed that, in the subsequent trials consisting in enlarging the models with additional input and output variables, grade of high-silica sand (main fraction) will be one of the inputs most intensively acting on the forecast mechanical and technological parameters of moulding sands hardened with microwaves. This thesis can be confirmed by weight fraction of this component in loose self-hardening moulding sands. Input data of the model were based on the examined sandmixes with weight fraction of the base from 94% to even 98%. Similarly, the main fraction of sands is of a great importance for permeability of the prepared sandmixes.

The next ones, with regard to their importance to the training process for the case of $MLP_1$ 10-6-2, were successively: the quantitative variable U1 responsible for the amount of water-glass added to the sand and the qualitative variable U11 coding by means of average module of the binder. In this model, effect of a binder content in the sandmix was stronger than effect of its average molar module. The suggested $MLP_1$ network, in spite of high matching (Table 5), changes in some way the traditional criteria of selection sequence of individual components of a sandmix.

In the cases of $MLP_2$ 10-5-2 and $MLP_3$ 10-6-2, more important for the training process were the qualitative variables U12 (coding acc. to percentage of oxides) and U13 (coding acc. to average density of the binder) that the quantitative variable U1 responsible for the amount of water-glass added to the moulding sand. In the $MLP_2$ and $MLP_3$ networks, sequence of selecting components of sandmixes in order to predict their properties referred to the traditional approach in that grade of the binder is decided first, and than its content in the sandmix.

## 5. Conclusions

The following conclusions can be drawn on the grounds of analyses of preliminary research on the possibility to predict mechanical and technological properties of microwave-hardened moulding sands containing water-glass:

- In comparison to linear and non-linear models describing effects of heating with electromagnetic waves, artificial neural MLP networks enable better matching of mathematical models and complex forecasting properties of moulding sands, like tensile strength and permeability.
- The MLP models demonstrate the expected, repeatable sensitivity to individual input variables in the training and validation sets, which proves their correctness.
- In all the analysed MLP networks, kind of high-silica sand (main fraction) most intensively affects training process of the mathematical model, which is confirmed by real observations of the manufacturing process of high-silica moulding sands.
- Depending on the way of coding individual properties of binders, it is possible a change of sensitivity of the network to the parameter of binder content in moulding sands.
- At the present stage of creating a mathematical way of forecasting parameters of sandmixes, the most desirable, with respect to the criterion of simplicity, protecting the network from overtraining, is the artificial neural network MLP 10-5-2 with the smallest hidden layer with activation of neurons in the layers by a hyperbolic tangent function.
- The generated and analysed artificial neural MLP networks make a basis for further searching of the models enabling the best complex forecasting of the basic parameters of sandmixes.

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