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# Modelling of hydrochemical and hydromechanical parameters' synergism in the process of solid deposit creation in geothermal and other hard waters

DRAGAN B. MILIĆEVIĆ[1]*, LJILJANA N. ANĐELKOVIĆ[2], MARJAN P. MITIĆ[2], JELENA M. PURENOVIĆ[3] and MILOVAN M. PURENOVIĆ[4]

[1]*University of Niš, Faculty of Civil Engineering and Architecture, Niš, Serbia,* [2]*University of Priština, Faculty of Technical Sciences, Kosovska Mitrovica, Serbia,* [3]*University of Kragujevac, Faculty of Technical Sciences, Čačak, Serbia and* [4]*University of Niš, Faculty of Science and Mathematics, Department of Chemistry, Niš, Serbia*

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*Abstract*: This paper presents the experimental research results, regarding the effect of hydromechanical parameters and based on the relative reduction of the starting hardness of geothermal water of Sijarinska Banja and Niška Banja as well as the water from the Medijana spring in Niš. The measurements were conducted on a laboratory pilot plant/ facility with glass pipes of diameter 2, 4, 6, 8 and 10 mm and with water flow controlled by a digital peristaltic pump with a flow interval from 2 to 5000 ml min$^{-1}$. The effect of the hydrodynamic parameters on the change of input hardness of geothermal and other hard waters and the process of solid deposit creation were modelled by an empirical model based on simple linear regression analysis, multiple linear regression model and the neural network. The high accuracy of all applied models unequivocally proves that a synergism of hydrochemical and hydrodynamic parameters exists in the process of creation of solid deposit – limescale, thanks to which the starting hypothesis is confirmed.

*Keywords*: water hardness; deposit and scale formation; hydrochemical and hydromechanical parameters.

## INTRODUCTION

Geothermal, underground and other waters of high mineralization and great hardness, present a complex composite heterogeneous system, which plays a very important role, especially in the distribution of such waters to the user. Whether it is the use of the waters in question in spa resorts and rehabilitation objects, or in a boiler or in other heating or cooling systems, it is surely not possible to prevent the formation of solid deposit – limescale.[1] Deposit in these systems reduces

* Corresponding author. E-mail: dragan.milicevic@gaf.ni.ac.rs
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the passage of heat, which increases the energy consumption, creates the conditions for corrosion under deposit, reduces the water flow velocity and disrupts the hydrodynamic regime, which leads to the decreasing of capacity of the entire system.[2]

There have been a plenty of reasons for solid deposit formation, because of the distinctively high mineralization of those waters with calcium and magnesium salts. From a chemical point of view, the synergy and presence of certain impurities in dissolved and colloid state have been clarified. This research will not consider the hydrochemical parameters of balance disruption of calcium and magnesium bicarbonates,[3] namely the changes which lead to the formation of the carbonate anion $CO_2$ firstly and later the carbonates of calcium and magnesium ($CaCO_3$ and $MgCO_3$) and the appearance of the solid deposit formation phenomenon – limescale, but it will analyse the effect of parameters on solid deposit formation – limescale.

In practice, it has been noted that limescale forms in heat supply or water supply systems where the water flow velocity is the smallest, in pipelines of small pipe diameter, or in places where water flows quite slow. This fact indicates that in the analysis of the causes of compact solid deposits, hydromechanical parameters cannot be bypassed, among which, except for the linear velocity of water flow, a probably important part belongs to flow criteria and pipe diameters, through which the flow process takes place. The research is based on a hypothesis that in the process of solid deposit – limescale formation a synergism of hydrochemical and hydromechanical parameters is present, and as a general hydrochemical parameter, the change of the input water hardness is observed.

The basic idea of the research is that the pilot facility, supplied with a peristaltic pump with a digitally regulated flow through a set of pipes of various diameters, enables a clip flow of geothermal and other hard waters and after that, through a change of real hardness, the effect of hydrodynamical parameters on the process of formation of solid deposit – limescale is observed. The research on the effects of hydromechanical parameters on the relative decrease of starting hardness have been conducted on samples of geothermal water of Sijarinska Banja and Niška Banja and water from the spring Medijana, Niš.[4] The analysis of the received experimental results in the past research was completed individually for each of the geothermal and other hard waters used in the research.[1,4] The received results have unequivocally confirmed the existence of a linear connection between the relative mass output flow of hardness, namely the relative change in hardness per unit of time on the exit of the pipe and the linear velocity, for different pipe diameters.[1] For each of the geothermal and other hard water used in research, a family of lines was received. That family of lines represents the dependence of mass output flow of hardness on the linear velocity for different pipe diameters.[1]

In this paper, we will analyse the received experimental results in research of hydromechanical parameter effects on the change of hardness of geothermal and other hard waters with different flow velocities on different glass pipe cross sections, in the direction of generalizing results, independently of the origins of the geothermal and other hard waters.

The results of this research should answer some disputable questions of theoretical character with the useful suggestions for practice and design of the systems for distribution of geothermal, underground and other hard waters.

## EXPERIMENTAL

*Materials and methods*

In order to measure the effect of hydromechanical parameters on the change of water hardness of geothermal and other hard waters and the process of solid deposit formation, water samples from Sijarinska Banja, off the Aragon spring, from Niška Banja, and off the drinking water spring Medijana were taken. The waters of Sijarinska and Niška Banja contain metasilicic and metaboric acid in considerate amounts, and the water from the Medijana spring contains the mentioned substances in very small quantities[4]. The water of Sijarinska Banja belongs to the category of sodium-hydrocarbonate, sulfide hypertherms, while the water of Niška Banja belongs to the category of slightly radioactive, calcium magnesium hydrocarbonate, oligomineral homeotherms.

*Laboratory pilot installation*

For realization of the predicted program and the research methodology, a pilot facility was planned (Fig. 1). The pilot facility consists of a set of glass pipes, 1000 mm of length whose diameters are 2, 4, 6, 8 and 10 mm. All of the pipes are made by extraction of Pyrex glass, so that the same conditions of roughness are created on the inner walls on all pipes. The flows and linear speeds are defined by a digital peristaltic pump DOSE – IT P910, IBS Integra Biosciences AGCH 7000 Chur Switzerland with water flow ranging from 0.6 to 5000 ml $min^{-1}$. The water temperature in the receiving reservoir with heater is controlled with the help of a thermostat with a constant temperature of 40 °C. In front of the pipe set a glass splitting dish is placed, whose volume is designed. It even allows flow through the system at high flow

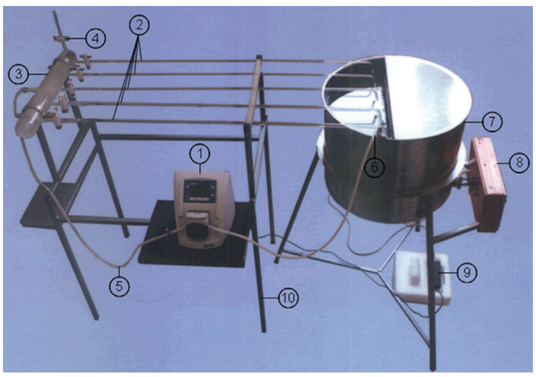



Fig. 1. Pilot installation for hydraulic investigation of linear flow velocity of geothermal and other hard waters and other hydromechanical parameters influence on solid deposits formation;[4] 1 – peristaltic pump, 2 – set of different diameters pipes, 3 – distribution splitting dish, 4 – degassing valve, 5 – silicon hose of the peristaltic pump, 6 – vacuum part of the peristaltic pump silicon hose, 7 – intake prochrome 80 l reservoir with heater, 8 – dashboard with thermostat and switcher, 9 – electrical energy supply, 10 – metal supporting frame.

rates. On the splitting dish, a venting valve is placed, so that the creation of a gas phase in the solid - liquid system is avoided at a piston flow through the glass pipe set.

*Experimental procedure*

Immediately before the experiment the examined water sample is filtered through blue ribbon paper and the starting water hardness is determined by the standard methodology. The water is poured into the open water heater, 80 $dm^3$ of volume, and the water is heated to 40 °C. For a pipe of the chosen diameter the given flow is adjusted. The taps on the other glass pipes are shut so that water flows only through the pipe of the chosen diameter with a steady flow. After the passing of constant time of 2 h, the pump is stopped, the water sample is taken, filtered through the blue ribbon and the residual hardness is measured by the standard method. At the end of the examination, for the pipe of the chosen diameter with single flow and finished measuring of residual water hardness, it is preceded to measuring on the same pipe but with different flows. After that, the same process as described is repeated for the remaining glass pipes out of the set. That way, the starting and final water hardness is determined for all pipe diameters and assigned flows.

*Analysis of experimental results*

*Analysis of results with use of the multiple linear regression model*. The dependence of a single occurrence on two or more independent occurrences can be examined with multiple regression, whose task is to find as many factors (independent variables) which have an effect on the examined occurrence (dependent variable) as possible. It is very important to carefully choose the variables which will be included in the model.

The model of multiple linear regression with n variables can be written as:

$$y = a_0 + a_1x_1 + a_2x_2 + a_3x_3 + ... + a_nx_n + \varepsilon \qquad (1)$$

where: $y$ – dependent variable; $x_1$, $x_2$,..., $x_n$ – independent variables; $a_0$ – intercept; $a_1$, $a_2$, ..., $a_n$ – regression coefficient; $\varepsilon$ – latent variable (accidental error).

This model gives the best possible prediction of values of the dependent variable for any combination of values of independent variables, if all assumptions are completed. The assumptions on which the multiple regression model is based on are the following: between the variables exists a linear dependence, which is especially important for the relation of independent variables with the dependent variable, multicollinearity between variables is small or nonexistent, all variables are continuous and have a variation interval, dispersion or a variance that makes sense, meaning that the most of the observations are not a single variation or interval and that in the base there is at least three to five times more observation data than there are variables, because otherwise the regression coefficients would be unreliable.

Based on sizes of the regression coefficients, it could be assumed what the relative effect or importance of each independent variable in the explanation of variations of the dependent variable is, or which volume of change of the dependent variable could be expected for each unit of change of each independent variable.

Multiple regression also show, through the correlation index $R$, how strong the correspondence of the dependent variable with all independent variables is, and through the determination index, $R^2$, how well the independent variables combined explain the variations, or how a reason could be assigned to them for the variation of the dependent variable and what is the percentage of variability of the dependent variable explained by the variability of independent variables.

Before the explanation of multiple regression results, testing of their statistical importance is needed. If the free form and all regression coefficients, $a_i$ ($i$ = 0,1,2,...,$n$) are statistically important, then the correlation index, $R$, will surely be important. Vice versa that does not have to happen because it is possible that because of a large number of variables a statistically important $R$ is received, and that coefficients $a_i$ ($i = 0,1,2,...,n$) are not important. If the free form and the regression coefficients, $a_i$ ($i = 0,1,2,...,n$) and the correlation index, $R$, are not statistically important, it is concluded that none of the independent variables have a real connection with the dependent variable, or that the received model has no practical value.

In practice, for describing physic-chemical processes a model of multiple linear regression with $n$ variables without the intercept, $a_0$ is used, if leaving out the intercept has no effect on the model relevancy, because the existence of a intercept is most often opposite of the physical reality, and the linear regression model with an intercept does not correctly describe the modelled processes.

*Data analysis with use of the neuron network*. The interest in the neuron network concept has increased over the last few years,[5] because of the ability to predict models based on neuron networks along with their adjustability.[5] The basic advantage of modelling with the use of neuron networks is the fact that it is enough to have the data on the input and output parameters with adequate training of the network to successfully generalize a model of satisfactory accuracy which enables precise prediction of output values for a new set of input data.[5] This advantage led to a wide application of neuron networks in various engineering disciplines.[5]

For application of this concept on modelling of chemical and biochemical processes usually the feed forward neuron network with a back propagation algorithm is used, composed of three elementary neuron layers; input, hidden and output. The number of neurons in the input layer is defined by the number of independently variable parameters, and the number of neurons in the output layer is defined by the number of dependently variable parameters, the prediction of which is wanted. There are no set rules to choose the optimal number of neurons in the hidden layer, or namely the optimal configuration of the neuron network. The number of neurons in the hidden layer is determined by the experience or the trial and error process.[5]

In the procedure of examining the influence of the change in the number of neurons in the hidden layer, the following recommendations can be applied on the quality model to select the range of variation of their number:[5]

$$nm = \sqrt{n+m} + a \tag{2}$$

$$\frac{N}{TW} \geq 1 \tag{3}$$

where: $n$ – number of input variables, $m$ –number of output variables, $a$ – parameter which changes from 1 to 10, $N$ – the total number of points used in modelling and $TW$ – total number of synaptic weights in the neuron network

After choosing the number of hidden neurons in the network and optimal configuration of the network, a choice of learning algorithm and its parameters is made. The choice of a learning algorithm, which sets the strengths or the synapse weights between certain neurons depends on the possibility of its application, relying on the difference in the nonlinearity of the observed problem.

During the training of the neuron network of the chosen configuration, the synaptic weights of certain neurons are changed with the aim of minimizing the mean squared error of data meant for the training, simultaneously the mean squared error of the data meant for check-up is calculated and when it starts to increase the training of the network is stopped.[5]

The result of the neuron network model can be interpreted through the interpretation of the output result, the interpretation of weights in the network, and sensitivity analysis (interpretation of importance of the input variables).

In most cases, the aim of training of the neuron network is to receive the smallest possible mistake for the value of the dependent variable calculated by the model in relation to experimental values of the dependent variable. As a measure of adequacy of the experimental result reproduction the mean squared error, *MSE* is used most often:

$$MSE = \frac{1}{n}\sum_{j=1}^{n}\left(P_{ij} - P_j\right)^2 \tag{4}$$

where: $P_{ij}$ – value of dependent variable received by neuron network calculation, $P_j$ – experimental value of the dependent variable and $n$ – number of experiments.

For the best match the *MSE* tends towards 0, when the calculated values completely match the experimental values of the dependent variables. It should be noted that in practice a rule on the size of the error which could be generally applied does not exit.[5]

Since the weights in the network are in certain an indicator of the importance of variables in the neuron network, analysis of their values after the network training phase proves useful. Greater values of the weights show that values of a certain variable in the network have a bigger influence on the calculation of the output value.

## RESULTS AND DISCUSSION

Table S-I of the Supplementary material to this paper shows the results of examination of hydromechanical parameter effects on the change of hardness of geothermal and other hard waters and the solid deposit formation process for geothermal water of Sijarinska Banja and Niška Banja and water from Medijana spring, completed according to the previously described experimental procedure.

The beginning and final water sample hardness for each pipe section and flow are determined experimentally. For each pipe diameter $D$ / mm and the corresponding pipe section, $A$ / mm$^2$ and flow $Q$ / L min$^{-1}$, a linear water velocity, $\upsilon$ / m s$^{-1}$ and Reynolds number, *Re*, are calculated, along with the flow rate multiplied by a ratio of output and input hardness, $G_0$ / L min$^{-1}$ expressed through the relative change of the input hardness, $C_i$ / mg L$^{-1}$ as $CaCO_3$ per unit time on the exit, according to the formula:

$$G_0 = \frac{C_0}{C_\mathrm{i}}Q \tag{5}$$

### *Experimental results modelling*

With the goal of confirming the starting hypothesis, the effect of hydrodynamic parameters on the change of input hardness of geothermal and other hard waters and the process of solid deposit formation are modelled by an empirical model based on simple linear regression analysis, the multiple linear regression model and the neuron network model.

The aim of the relatively simple empirical model based on simple linear regression analysis is to define which hydromechanical parameter has an effect on the change of input hardness of geothermal and other hard waters, and to establish the functional dependence between them, while the goal of the more complex model of multiple linear regression and the neuron network model is to verify the established functional dependence of hydrochemical and hydromechanical parameters in the solid deposit formation process, which will verify the starting hypothesis.

For calculation of linear regression models the DataFit v8.1.69 software by Oakdale Engineering was used and for the neuron network model development the MatLab R12 software by MathWorks was used.

It should be mentioned that all models which are presented in this paper are valid only for the range of experimental data used for modelling and for water temperature of 40 °C, on which experimental measuring was performed.

*Empirical model based on linear regression analysis*

The appropriate calculated relative mass flows of output hardness, $G_0$, and linear velocity, $\upsilon$ (Table S-I), are grouped for each pipe diameter, $D$, and are individually fitted with a single linear regression model without a free form, which can be shown with the formula:

$$G_0 = a\upsilon \tag{6}$$

where: $a$ – linear regression coefficient.

The linear regression model dependences of the relative mass flow of hardness from the linear velocity for different pipe diameters is shown in Table I.

TABLE I. Parameters of the linear regression model for different pipe diameters

| $D$ / mm | $a$ | Linear regression model | $R^2$ | Standard error of the estimate |
|---|---|---|---|---|
| 2 | 0.19155 | $G_0 = 0.19155\upsilon$ | 0.9973 | 0.033 |
| 4 | 0.77285 | $G_0 = 0.77285\upsilon$ | 0.9979 | 0.030 |
| 6 | 1.70469 | $G_0 = 1.70469\upsilon$ | 0.9822 | 0.079 |
| 8 | 3.00524 | $G_0 = 3.00524\upsilon$ | 0.9887 | 0.054 |
| 10 | 4.72197 | $G_0 = 4.72197\upsilon$ | 0.9677 | 0.088 |

The values of the correlation coefficient, $R^2$, is close to 1 and small values of the standard error of the estimate for the defined regression models for all pipe diameters (Table I), unequivocally affirm that a strong linear connection exists between the relative mass flow, that is the relative change of hardness per unit time on the exit, and the linear velocity, for different pipe diameters, for the examined geothermal and other hard waters, are independent from their origin. The received linear regression models for different pipe diameters for the examined geothermal and other hard waters are shown on Fig. 2.

As can be seen in Fig. 2, families of straight lines which represent the dependences of the relative mass flow of hardness on the output from the linear velocity for different pipe diameters are received.

With further analysis it was established that a connection between the regression coefficient, $a$ in formula (6) and the square of the pipe diameter, $D^2$, are shown in Table I, and that the connection can be the best defined by a single linear regression model without a intercept:

$$a = bD^2 \tag{7}$$

where: $b$ – linear regression coefficient.

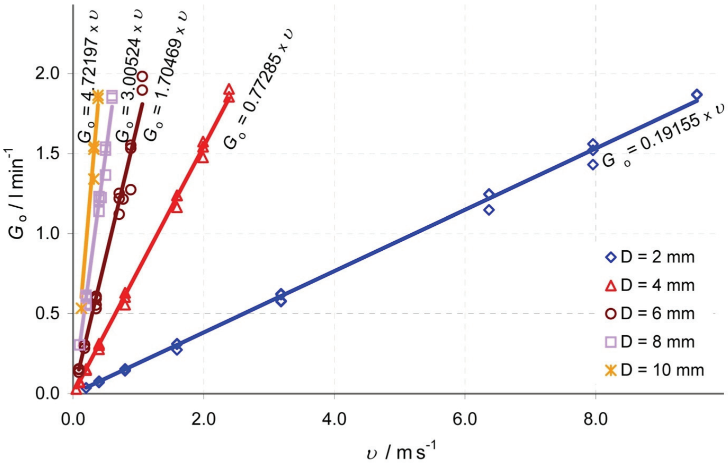



Fig. 2. Dependences of relative mass flow of hardness on the exit on the linear velocity for different pipe diameters.

A single linear regression model (7) of dependence with coefficient, $a$, in formula (6) and square of pipe diameter, $D^2$, is received in the form:

$$a = 0.0472D^2 \tag{8}$$

For which the correlation coefficient is $R^2$ = 0.99996 and standard error of the estimate = 0.01214, which shows that the model is highly accurate and confirms a very strong connection between the regression coefficient value, $a$, in formula (6) and square of the pipe diameter, $D^2$.

Based on the formulas (6) and (8), the relative mass flow of output hardness can be defined by the formula:

$$G_0 = 0.0472\,\upsilon\,D^2 \tag{9}$$

Based on the formulas (5) and (9) the output hardness can be defined by the empirical model:

$$C_0 = 0.0472 C_\mathrm{i} \frac{\upsilon}{Q} D^2 \tag{10}$$

The received empirical model, based on single linear regression analysis of experimental results, is highly accurate ($R^2$ = 0.99658, standard error of the estimate = 4.34177, *MSE* = 18.851).

Regarding that $\upsilon$ and $Q$ are co-dependent variables, based on the empirical model (10), it can be concluded that the variability of the output hardness, $C_0$ for different variations of input influential parameters ($C_iQD^2$), which confirms the functional dependence of the output hardness, $C_0$ is not just dependant on the input hardness, $C_i$, but also from the hydrodynamical parameters, specifically the linear pipe flow, $Q$, and square of pipe diameter, $D^2$, meaning that:

$$C_0 = f(C_iQD^2) \tag{11}$$

The defined functional co-dependence (11) confirms the starting hypothesis that in the process of hard deposit formation – limescale, exists a synergism of the change of input water hardness, as an adopted primary hydrochemical parameter and hydromechanical parameters, specifically pipe flow and pipe diameter.

*Model of multiple linear regression with three independent variables*

For the analysis of the influence the hydrodynamical parameters have on the change of hardness of geothermal and other hard waters and the process of solid deposit formation, a model of multiple linear regression with three independent variables, can be written, based on formula (1) and the defined functional dependence (10), in the form:

$$C_0 = a_0 + a_1C_i + a_2Q + a_3D^2 \tag{12}$$

Results of the regression analysis for the adopted model of multiple linear regression with three independent variables are shown in Table II.

The results presented in Table II show that the multiple linear regression model with three independent variables describes the experimental data very well and the connection between the variables is quite strong. The coefficient of multiple determination, $R^2$ equals 0.9970, meaning that the model explains 99.70 % of variability of the output hardness for different values of input parameters. The standard error of the estimate, which shows the standard deviation of residuals, equals 3.76911. The residual sum of squares, which shows the sum of squares of the difference between the experimental data and the data, generated by the regression model equals 1065.46592, and finally the mean square error, *MSE*, which shows the adequacy of the experimental result reproduction equals 14.206.

The first regression coefficient, $a_1$, is interpreted as an increase of the output hardness, $C_0$, by 0.99969 mg $L^{-1}$ as $CaCO_3$ if the input hardness, $C_i$ increases by 1 mg $L^{-1}$ as $CaCO_3$, and the remaining independent variables stay unchanged, the second regression coefficient, $a_2$, is interpreted as an average decrease of the output hardness, $C_0$, by –2.66662 mg/l $CaCO_3$ if the flow, $Q$ increases by 1 L $min^{-1}$, and the remaining independent variables stay unchanged, and the fourth regression coefficient is interpreted as an average increase of the output hardness,

$C_0$ by 0.02490 mg L$^{-1}$ as $CaCO_3$ if the square of the pipe diameter, $D^2$, increases by 1 mm, and the remaining independent variables stay unchanged. It can be concluded that the output hardness, $C_0$, is in direct proportion with the input water hardness, $C_i$, and the square of the pipe diameter, $D^2$, but inversely proportional to the pipe flow, Q.

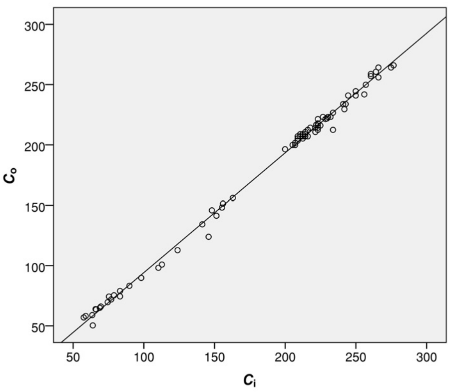
TABLE II. Results of regression analysis for the multiple linear regression model with three independent variables

| | | | | | |
|---|---|---|---|---|---|
| Sum of Residuals = 2.47581510848249E-10 | | | | | |
| Average Residual = 3.1339431752943E-12 | | | | | |
| Residual Sum of Squares (Absolute) = 1065.46592144379 | | | | | |
| Residual Sum of Squares (Relative) = 1065.46592144379 | | | | | |
| Standard Error of the Estimate = 3.76911293090526 | | | | | |
| Coefficient of Multiple Determination (R^2) = 0.9969843461 | | | | | |
| Proportion of Variance Explained = 99.69843461% | | | | | |
| Adjusted coefficient of multiple determination (Ra^2) = 0.99686372 | | | | | |
| Durbin–Watson statistic = 2.02209675423985 | | | | | |
| Regression variable results | | | | | |
| Variable | Value | Standard error | *t* Ratio | *Prob*(*t*) | |
| $a_0$ | –4.88548 | 1.36644 | –3.57534 | 0.00062 | |
| $a_1$ | 0.99969 | 0.00667 | 149.89886 | 0.00000 | |
| $a_2$ | –2.66662 | 0.77606 | –3.43611 | 0.00097 | |
| $a_3$ | 0.02490 | 0.01632 | 1.52588 | 0.13124 | |
| Variance Analysis | | | | | |
| Source | *DF* | Sum of squares | Mean square | *F* Ratio | *Prob*(*F*) |
| Regression | 3 | 352246.274 | 117415.425 | 8265.076 | 0 |
| Error | 75 | 1065.466 | 14.206 | | |
| Total | 78 | 353311.740 | | | |

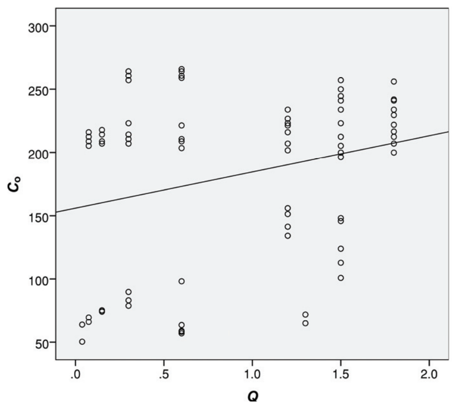
The estimated intercept $a_0$ and the regression coefficients $a_1$ and $a_2$ have high values of the $t$ ratio ($t$ ratio$_{a_0}$ = –3.57534 > $t_{0.05}(75)$ = 1.667, $t$ ratio$_{a_1}$ = 149.89886 > $t_{0.05}(75)$ = 1.667 and $t$ ratio$_{a_2}$ = –3.43611 > $t_{0.05}(75)$ = 1.667), and small values of *Prob*($t$) (0.00062, 0 and 0.00097), which indicates that there is no possibility that their values can be zero, meaning that these regression coefficients are statistically important and cannot be removed from the regression model without decreasing the validity of the model.

The estimated regression coefficient $a_3$ has a relatively low value of the $t$ ratio ($t$ ratio$_{a_3}$ = 1.52588 > $t_{0.05}(75)$ = 1.667 and a relatively high value of *Prob*($t$) (0.13124), which indicates that a small possibility exists (13.12 %) that the coefficient value can be zero.

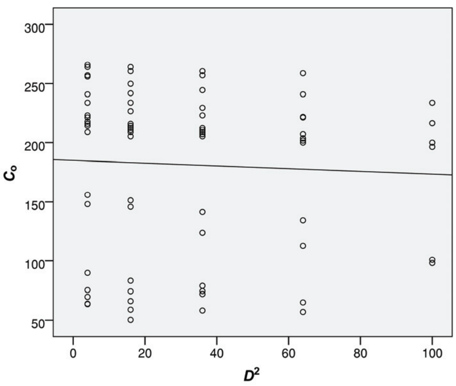
The high quality of the applied regression model is shown in the regression model diagram presented in Fig. 3 where it can be seen that the data are randomly distributed above and below the regression plane and that the applied model adjusts well to the experimental data.




(a)




(b)




(c)

Fig. 3. Scatter plots of multiple linear regression model results; scatter plot of input $C_i$ and output hardness $C_0$ (a); scatter plot of flow $Q$ and output hardness $C_0$ (b); scatter plot of square of the pipe diameter $D^2$ and output hardness $C_0$ (c).

It can be concluded that the received results make statistical and scientific sense, and that the values of certain variables are not opposite to the physical reality, meaning that the multiple linear regression model with three independent variables correctly describes the modelled processes. The received model is highly accurate and it can describe the variability of the output hardness, $C_o$ for different variations of the influential input parameters ($C_iQD^2$) well, which confirms the starting hypothesis and the functional dependence (11) of the output hardness, $C_0$ from the input water hardness, $C_i$ and hydrodynamical parameters: pipe flow, $Q$, and the square of pipe diameter, $D^2$.

*Results of the neuron network model with three independent variables*

Since the neuron network model based on the defined functional dependence (11) should mould the influence of the three independent variables, namely the input values ($C_iQD^2$) on a single dependent variable, namely the output value, $C_0$, the number of neurons in the input layer, will equal 3 and in the output layer will equal 1. Although the aim of this paper was not the choice of the optimal neuron network configuration for its use in the modelling of the solid deposit formation process, with the use of recommendations defined by formula 2 the number of neurons in the hidden layer is varied from 3 to 12, with the satisfied condition defined by formula (3) that the $N/TW$ ratio is larger than one.

In the used software package there are more defined learning algorithms, and in this paper for all configurations of the neuron network one of the most common algorithms in literature was used.[5] It was the Levenberg–Marquardt method (trainlm – MATLAB network training function), with an adopted degree of the learning rate from 0.25 and the neuron network momentum coefficient for the chosen learning algorithm of 0.5.

For its application in modelling the change of hardness of geothermal and other hard waters and the solid deposit formation process, the experimental data (Table S-I) are separated into three groups in the used software: the data for learning, the data for check-up and the data for testing of the neuron network.

In the analysis of the optimal neuron network configuration, it was proved that the increase of the number of neurons in the hidden layer leads to an improvement in the predictable properties of the neuron network. With an increase of the number of neurons, the mean square error decreases and has the lowest value when the number of neurons equals 9. Further increase of the number of neurons does not contribute to the improvement of the network prediction, so the adopted networks configuration is the configuration with one hidden layer of 9 neurons, or 3-9-1 neurons. The results of moulding the experimental data with the neuron network model with an adopted configuration of 3-9-1 neurons and an adopted learning algorithm are shown in Fig. 4.

As it was assumed, during the training of the neuron network on the experimental data, the neuron network model could adequately show the change of hardness of geothermal and other hard waters as well as the process of solid deposit formation depending on the hydrodynamical parameters.

The received values of the correlation coefficient, $R$, of 0.99916, or the determination coefficient, $R^2$, of 0.9983 point to the great agreement of the experimental data and the data received with the neuron network model, based on the set experimental data for learning.

The models received by the application of the neuron network methodology typically have a great prediction value on the set of data for learning, and a significantly smaller value on the test set of data or on the set of new, unknown data.[5] However for the neuron network model with the adopted configuration of 3-9-1 neurons and the adopted learning algorithm for the data set for check-up, the data set for testing of the neuron network, as well as the complete set of experimental data the received values of the correlation coefficient, $R$, of 0.99907, 0.99544 and 0.9988 or the determination coefficient, $R^2$, of 0.99814, 0.99090 and 0.99760, respectively, indicate the good correlation of the experimental data and the data received by the neuron network model.

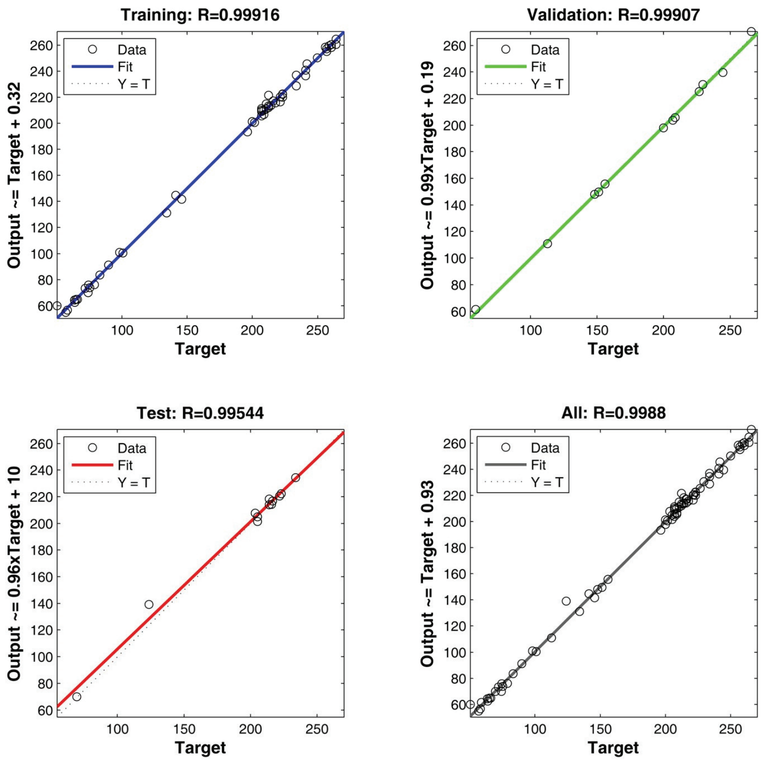



Fig. 4. Neural network model regression.

The received neuron network model has a very high accuracy and it can describe the variability of the output hardness, $C_0$ for different variations of the influential input parameters ($C_iQD^2$), which confirms the starting hypothesis and the functional dependence (10) of the output hardness, $C_0$ from the input water hardness, $C_i$ and hydrodynamical parameters: pipe flow, $Q$, and square of the pipe diameter, $D^2$.

For the exact application of the neuron network model in the moulding of the solid deposit formation processes in the observed range of data (Table S-I) it is sugessted a choice of the optimal neuron network configuration, the learning algorithm and its parameters (the learning rate and momentum coefficient) which will provide the highest accuracy of the system.

*Summary of experimental results modelling*

All applied models show that the connection between variables is very strong and describe the experimental data well, which is confirmed by the multiple determination coefficient, $R^2$, close to one in all models and the low value of the mean square error, *MSE*, which equals 18.851 in the empirical model, 14.206 in the multiple linear regression model, and 10.7903 in the neuron network model.

The accuracy of the applied models could best be shown by application of the model on the experimental data (Table S-I). In Fig. 5 the results of predictions of the experimental data for all applied models are shown.

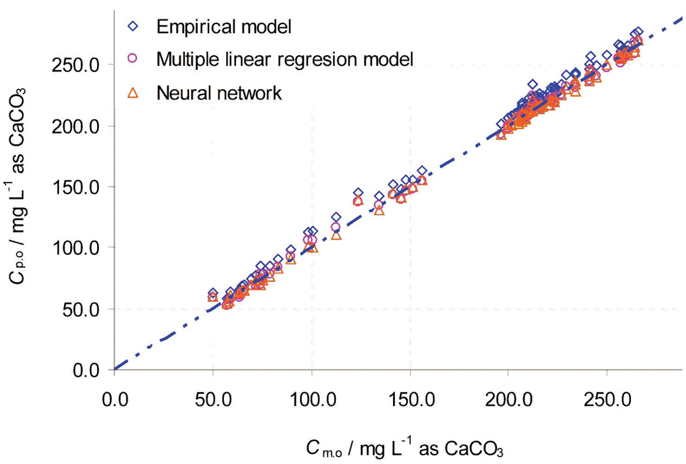



Fig. 5. Scatter plot of predicted and measured output hardness.

The diagram shown in Fig. 5 confirms the accuracy of the applied models because for all applied models the small dispersal of prediction values appears for the output hardness around the line of $C_{p.o} = C_{m.o}$, which represents the absolutely correct prediction, or that the prediction values of the output hardness, $C_{p.o}$ are very close to the experimentally determined values, $C_{m.o}$ for all applied models.

## DISCUSSION

In this research the changes of water hardness, as one of the hydrochemical parameters, are put in function of hydromechanical parameters, so that the insight could be received into the synergism between the hydrochemical and hydromechanical parameter in the solid deposit formation process.

The solid deposit formation process is highly complex and depends on the hydrochemical and hydrodynamical parameter. As a starting general hydrochemical parameter in this research, the input water hardness was adopted. The completed program and research methodology confirmed the set foundations and pointed towards the synergism model between the hydrochemical parameters of solid deposit formation and the hydrodynamical parameters.

With an empirical model based on single linear regression, the multiple linear regression model and the neuron network model with three independent variables, it was confirmed that except the linear velocity as an independent variable, there are also other independent variables which influence the change of the input hardness, as the dependent variables in the solid deposit formation process. In all applied models, the output hardness, $C_0$ was coupled as a dependent variables with four independent variables: input hardness, $C_i$; pipe flow, $Q$ and square of pipe diameter, $D^2$. The applied models describe the experimental data well, and the connection between the variables is very strong, which is confirmed by the multiple determination coefficient, $R^2$ close to one and a small value of the mean square error, *MSE* in all models.

The quality of the applied models unequivocally confirms that a multiply defined synergism of the hydrochemical and the hydrodynamical parameters exists, which in turn confirms the starting hypothesis and creates a starting point for a more variable analysis of the complex phenomena of the solid deposit formation and the explanation of the processes happening in the heterogeneous solid-liquid system.

## CONCLUSION

The basic indicator of the alternation of the hydrochemical parameters is the change of hardness which is followed by the different flows and the different flow velocities through the glass pipes of various intersections. By modelling the experimental data, with the use of different model types expected changes of hydrochemical parameters, were observed on the influence of hydromechanical parameters. The empirical model based on the single linear regression analysis, the multiple regression model and the neuron networks model with three independent variables includes hydromechanical parameters: pipe flow and pipe diameter. Results of all applied models have shown a very high value of the multiple determination coefficient, $R^2$ close to one, with a small standard error and they have confirmed a good adaptability of the mathematical model to the experimental data. With the high accuracy of all applied models it was unequivocally confirmed that a multiply defined synergism exists between the hydrochemical and the hydrodynamical parameters in the solid deposit – limescale formation process, which in turn confirms the starting hypothesis.

The applied modelling describes the influence of the hydrodynamical parameters well, and the connection with the change of water hardness enables an all encompassing view of the synergism of the hydrochemical and the hydromechanical parameters.

SUPPLEMENTARY MATERIAL

Results of completed examination for geothermal water are available electronically at the pages of the journal website: http://www.shd.org.rs/JSCS/, or from the corresponding author on request.

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ИЗВОД

МОДЕЛОВАЊЕ СИНЕРГИЗМА ХИДРОХЕМИЈСКИХ И ХИДРОМЕХАНИЧКИХ ПАРАМЕТАРА У ПРОЦЕСУ СТВАРАЊА ЧВРСТИХ ДЕПОЗИТА У ГЕОТЕРМАЛНИМ И ДРУГИМ ТВРДИМ ВОДАМА

ДРАГАН Б. МИЛИЋЕВИЋ[1], ЉИЉАНА Н. АНЂЕЛКОВИЋ[2], МАРЈАН П. МИТИЋ[2], ЈЕЛЕНА М. ПУРЕНОВИЋ[3] и МИЛОВАН М. ПУРЕНОВИЋ[4]

*1Универзитет у Нишу, Грађевинско-архитектонски факултет, Ниш, [2]Универзитет у Приштини, Факултет техничких наука, Косовска Митровица, [3]Универзитет у Крагујевцу, Факултет техничких наука, Чачак и [4]Универзитет у Нишу, Природно-математички факултет, Департман за хемију, Ниш*

У раду су приказани резултати експерименталних истраживања утицаја хидромеханичких параметара на релативно смањење полазне тврдоће геотермалне воде Сијаринске бање и Нишке бање и воде из изворишта Медијана, Ниш. Експериментална истраживања су изведена на лабораторијском пилот постројењу са стакленим цевима пречника 2, 4, 6, 8 и 10 mm, на коме је проток контролисан дигиталном перисталтичком пумпом са интервалом протока од 2 до 5000 ml min$^{-1}$. Утицај хидродинамичких параметара на промену улазне тврдоће геотермалних и других тврдих вода и процес стварања чврстих депозита су моделовани емпиријским моделом базираним на простој линеарној регресионој анализи, моделом вишеструке линеране регресије и неуронском мрежом. Високом тачношћу свих примењених модела недвосмислено је потврђено да постоји вишеструко изражени синергизам хидрохемијских и хидродинамичких параметара у процесу стварања чврстих депозита – каменца, чиме је полазна хипотеза истраживања потврђена.

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