ISSN 1330-3651 (Print), ISSN 1848-6339 (Online)
https://doi.org/10.17559/TV-20210925112341
Original scientific paper

Gaussian Regression Process for Prediction of Compressive Strength of Thermally Activated Geopolymer Mortars

Nenad RISTIĆ*, Emina PETROVIĆ, Jelena BIJELJIĆ, Miloš SIMONOVIĆ, Dušan GRDIĆ, Vlastimir NIKOLIĆ, Zoran GRDIĆ

Abstract: The primary objective of this research is the development of a prediction model of the compressive strength of geopolymer mortars made with fly ash and granular slag which hardened in different curing conditions. Data for the numerical analysis were obtained by experimental research; for this purpose 45 series of geopolymer mortars were made, 9 of which were cured in ambient conditions at a temperature of 22 °C, and the remaining were exposed to thermal activation for a duration of 24 h at the temperatures of 65 °C, 75 °C, 85 °C and 95 °C. Using machine learning, a Gaussian regression method was developed in which the curing temperature and the percentage mass content of fly ash and granular slag were used as input parameters, and the compressive strength as the output. Based on the results of the developed model, it can be concluded that the Gaussian regression process can be used as a reliable regression method for predicting the compressive strength of geopolymer mortars based on fly ash and granular slag.

Keywords: curing temperature; fly ash; Gaussian regression process; geopolymer mortars; ground granulated blast furnace slag; machine learning

1 INTRODUCTION

Composites made from waste binders and aggregates are environment friendly mixtures and they are a relatively new concept in the field of materials. A special attention in the field of environmentally friendly building composites is attracted by geopolymers which are considered to be third generation materials and are defined as a subgroup of alkali-activated materials [1]. The mechanical properties of geopolymers directly depend on the characteristics of the starting materials [2], concentration and quantity of alkali solutions [3], but also on the implemented curing regime [4-5]. A slow development of initial strengths in ambient conditions, as well as somewhat more complex production technology in comparison to the cement composites are the basic reasons for the small market share of geopolymer composites [6]. Accelerated hardening of geopolymers, and thus accelerated development of strengths, can be provided by thermal activation, i.e. exposure of geopolymers to elevated temperatures in a certain time interval. Adam and Horanto [7] concluded that duration and curing temperature have influence on strength of geopolymer paste. According to them, the highest strengths of geopolymers were achieved when samples were exposed for 20 h to a temperature of 120 °C in a closed mould. Kumaravel [8] concluded that the compressive strength of geopolymer concrete cured in oven was higher than the strength achieved on ambient cured concrete. He found an optimum strength at 60 °C for a day. C. D. Atis et al. [9] investigated the effects of exposing geopolymer mortars to temperatures in the range 45 °C to 115 °C for 24 h, 48 h and 72 h on their strength. They concluded that the high temperature and the duration of the temperature effects had an impact on the development of mechanical strengths, and the highest strength was measured on samples of geopolymers exposed to temperatures of 115 °C for 24 h. There is a small number of studies in which comparative testing of the properties of geopolymer composites cured in ambient and high temperature conditions has been performed [10-14]. The general conclusion of the authors is that exposure of samples to elevated temperatures provides high early strengths, but their increase at later ages is negligibly small. On the other hand, in samples cured in ambient conditions, the increase in strength over time is slower, but the final values of strength are higher compared to geopolymer samples that were thermally activated.

Since in the geopolymer composites the connection between the mix design, curing regime and strength is complex [15], non-linear and depends on a number of factors, and the very preparation process increases the consumption of material, time, and human labor leading to a higher cost of the final product, this means that the mathematical methods for prediction can be of significance [16-17]. Most frequently used methods when modelling cement composites strength are mathematics statistical forecasting method and nonlinear prediction method. Yet, they did not prove to be suitable for geopolymer modelling. For this purpose, it would be convenient to use the numerical method which would form the relationship between the dependent and independent variables [16, 18-19]. Feeding the system with a set of input datasets of various mixtures would perform the prediction of output parameters [20]. Most of these papers use the neural networks (NN) for predicting and estimating the various characteristics of construction materials. Up to date, only a few authors tested geopolymers using mathematical models. Awoyera et al. [21] modeled the strength characteristics of SCC geopolymer by using genetic programming and artificial NN techniques. The authors develop the minimal errors prediction model with compressive strength, split-tensile strength and flexural strength parameters as a response. Bagheri et al. [22] employed artificial NN in order to create a function of compressive strength of boroaluminosilicate geopolymers. A model of high level of accuracy and reliability was obtained, where *R* squared and root mean square error were 0,95 and 0,07, respectively. Hybrid neural networks were also considered for predicting the compressive strength of geopolymer. In [17] an Adaptive neuro-fuzzy interface (ANFFIS) was constructed, trained, and validated to predict the compressive strength of geopolymer concrete where coarse and fine waste steel slag were used as an aggregate. Van Dao et al. [18] investigates a particle swarm optimization (PSO)-based adaptive network-based fuzzy inference system (PSOANFIS) and a genetic algorithm

(GA) based adaptive network based fuzzy inference system (GAANFIS), while *R* of tested models were 0,934 and 0,927, respectively. The multilayered NN were also considered as a promising tool for prediction of mechanical characteristics of geopolymers. In [16], the deep NN and deep residual NN were trained on a set of 355 samples in order to predict the compressive strength of geopolymers. The authors concluded that both models can be used to predict the compressive strength of geopolymers, yet with no normalization and no dropout the deep residual NN proved to be better. Other authors used analysis of variance on the results in order to assess the value of parameters of geopolymers [23]. In their research, M. Lahoti et al. [24] used machine learning-based classifiers to predict the compressive strength of metakaolin-based geopolymer mixes using both data obtained by testing and from the literature. As a result of this research, the authors state that the implemented machine learning method can be used to predict the strength of tested geopolymers of high precision. The major problem NN is faced with is overfitting. When the model is trained too specifically to the training data then it may not be so good in performing prediction. This can be a problem when a model has a quite large number of parameters and a low number of training data. Otherwise, it is possible to train the network even with an insufficient predictive capacity [25]. Also, some authors attempted other machine learning approaches to modeling such as the support vector regression technique in order to assume the strength behavior of ground granulated blast furnace slag (GGBFS) based geopolymer stabilized clayey soil [26]. The Gaussian processes regression (*GPR*) can also be used for regression and classification tasks [27] of geopolymers as the probabilistic supervised machine learning algorithm. As a non-parametric model, the *GPR* method can make predictions incorporating prior knowledge (kernels) and provide uncertainty measures over predictions and be used effectively even when an available data set is relatively small. Overfitting is generally not a concern in *GPR* and the biggest advantage of *GPR* is the ability to choose hyperparameters and covariances directly from the training data, using either a maximum likelihood or the Bayesian approach [28].

In this paper *GPR* models with different kernels for predicting mechanical characteristics were developed and tested. Experiments were done in a laboratory and the obtained input-target values were then used to train the regression models. The input data includes curing regime, percentage-masse content of fly ash (FA) and GGBFS while the target value is the compressive strength. The main focus of this research is to develop a compressive strength prediction model of geopolymers by using *GPR* when input data change.

2 GAUSSIAN PROCESS REGRESSION ALGORITHM

GPR is a machine learning method based on using mathematical concept from machine learning, optimisation, the Bayesian inference and statistical learning theory [29]. GRP is often called the nonparametric model, because it does not rely on a finite set of parameters [30]. From the function point of view the Gaussian process is defined as any set of finite random variables which have a joint (multivariate) Gaussian distribution Eq. (1):

$$f(x) \sim GP\left(\mu(x),\, k(x, x')\right) \tag{1}$$

In other words, *GPR* calculates the probability distribution over all acceptable functions that fit the data, rather than calculate the probability distribution of parameters of a specific function. The covariance function $k(x, x')$ is also known as a "kernel function" and it can be expressed in several differential forms. The kernel is parameterized by a set of kernel parameters commonly known as hyper parameters [31].

The joint distribution of the observed values $\boldsymbol{y}$ and the predicted values of the Gaussian process, $\boldsymbol{f^*}$ at the test points $\boldsymbol{x^*}$ are calculated as in Eq. (2):

$$\begin{aligned}\begin{bmatrix}\boldsymbol{y}\\ \boldsymbol{f}^*\end{bmatrix} &= N\left(\boldsymbol{0}, \begin{bmatrix}\boldsymbol{K}(\boldsymbol{x},\boldsymbol{x})+\boldsymbol{\sigma_n^2 I_n} & \boldsymbol{K}(\boldsymbol{x},\boldsymbol{x}^*)\\ \boldsymbol{K}(\boldsymbol{x}^*,\boldsymbol{x}) & \boldsymbol{K}(\boldsymbol{x}^*,\boldsymbol{x}^*)\end{bmatrix}\right) = \\ &= N\left(\boldsymbol{0}, \begin{bmatrix}\boldsymbol{K}+\boldsymbol{\sigma_n^2 I_n} & \boldsymbol{K_*^T}\\ \boldsymbol{K_*} & \boldsymbol{K_{**}}\end{bmatrix}\right)\end{aligned} \tag{2}$$

$K(x, x)$ denotes the $n \times n$ symmetric positive definite covariance matrix evaluated at all pairs of training points $\boldsymbol{x}$. $\boldsymbol{K(x, x^*)}$ denotes the covariance matrix of the new input test point $\boldsymbol{x^*}$ and all the training points $\boldsymbol{x}$, and $\boldsymbol{K(x^*, x^*)}$ denotes the covariance matrix evaluated at the test point x*. $\boldsymbol{\sigma_n^2}$ is the positive noise covariance and $\boldsymbol{I_n}$ is an identity matrix.

The conditional distribution of the predicted Gaussian process conditioned on the observed training outputs $\boldsymbol{y}$ is expressed as in Eq. (3):

$$\boldsymbol{f}^* \left| \boldsymbol{x}, \boldsymbol{x}^*, y \sim N\left(\overline{f^*},\, cov\left(f^*\right)\right)\right. \tag{3}$$

where: predicted value and test points $\boldsymbol{x^*}$ are given by:

$$\overline{f^*} = K\left(x, \bar{x}\right)\left[K(\boldsymbol{x},\boldsymbol{x})+\boldsymbol{\sigma_n^2 I_n}\right]^{-1}\boldsymbol{y} \tag{4}$$

and convergence:

$$cov\left(f^*\right) = \boldsymbol{K}\left(\bar{\boldsymbol{x}}, \bar{\boldsymbol{x}}\right) - \boldsymbol{K}\left(\boldsymbol{x}, \bar{\boldsymbol{x}}\right)\left[\boldsymbol{K}(\boldsymbol{x},\boldsymbol{x})\boldsymbol{\sigma_n^2 I_n}\right]^{-1}\boldsymbol{K}\left(\boldsymbol{x}, \bar{\boldsymbol{x}}\right)^T$$

So, it can be said, that the Gaussian process regression is defined by two functions: the mean function and the covariance function.

Based on the Bayes' theorem (Eq. (4)) the hyperparameters are usually computed by maximizing the marginal likelihood $\log p\left(\boldsymbol{y}|\boldsymbol{x}, \boldsymbol{\theta}\right)$.

$$\begin{aligned}\log p\left(\boldsymbol{y}|\boldsymbol{x}, \boldsymbol{\theta}\right) &= -\frac{1}{2}\boldsymbol{y}^T\left[\boldsymbol{K}+\sigma_n^2\right]^{-1}\boldsymbol{y} - \frac{1}{2}\log\left[\boldsymbol{K}+\sigma_n^2\right] - \\ &-\frac{n}{2}\log 2\pi\end{aligned} \tag{5}$$

where:$\boldsymbol{\theta}$ presents the values of the hyperparameters in the kernel.

3 EXPERIMENTAL PROCEDURE
3.1 Materials

In this study FA and GGBFS were used as the binder materials for making geopolymer mortars. FA originated from the thermal power plant Kostolac "B" (Serbia), created by burning the lignite ore, while GGBFS byproduct was created in the production of steel in the steelworks HBIS Group Iron & Steel (Serbia). For the needs of the test GGBFS was ground in a ball mill, and then passed through the sieve having mash opening of 90 µm. The same sieve was used to sift FA in order to remove coarse particles. According to the chemical composition provided in Tab. 1, the used FA belongs to the group of silicate ash, while GGBFS is classified as alkaline material.

Table 1 Chemical composition of used binders

Parameter	Fly ash / %	Ground granulated blast furnace slag / %
SiO_2	51,68	38,1
Fe_2O_3	11,58	0,7
Al_2O_3	20,16	7,17
CaO	7,43	39,48
MgO	2,41	9,86
SO_3	2,02	0,36
P_2O_5	0,12	-
TiO_2	1,04	-
Na_2O	0,88	0,51
K_2O	1,04	0,23
LOI	2,57	1,01

Physical properties, pozzolanic activity and the activity index of used FA and GGBFS are given in Tab. 2, while in Fig. 1 their SEM and photographs are displayed.

Table 2 Physical properties of used binders

Properties	FA	GGBFS	Requirement
Specific gravity SRPS B.C8.023 t.4.2 [32] / g/cm^3	2,24	2,85	-
Loose bulk density SRPS B. C8.023 t.4.3 [32] / g/cm^3	0,81	1,24	-
Color	grey	brown	-
Pouzzolanic activity SRPS B.C1.018:2015 [33] (Class)	10	5	Class 5: σ_f = 2 MPa, σ_c = 5 MPa. Class 10: σ_f = 3 MPa, σ_c = 10 MPa.
Activity index FA SRPS EN 450-1 [34] / %	97	-	28 days - 75%
	105		90 days - 85 %
Activity index GBFS SRPS EN 15167-1 [35] / %	-	60	7 days - 45%
		87	28 days - 70%

3.2 Mix Design

In order to determine the impact of the curing regime on the characteristics of geopolymer mortars, 9 different series of geopolymer mortar based on FA with GGBFS added were made. The percentage of GGBFS mass in respect to the total mass of the binder was 0 to 100%, in 12,5% steps of replacement. Each series consisted of 5 subseries, composed of 3 prisms having dimensions 40 × 40 × 160 mm.

After mortar samples were cast, the samples of 4 remaining mortar subseries were firstly cured at ambient temperature of 22 °C for 24 h in a mould covered with a glass plate (in order to prevent the moisture loss). After that the specimens were heated in the oven by using four different temperatures, started and ended heating proces with specifly choosed temperature. The temperature of curing was varied at an interval of 10 °C. The curing temperatures were 65 °C, 75 °C, 85 °C and 95 °C for 24 hours inside oven and then samples were tested. After the rest time for temperature activation elapsed, the samples of these mortar subseries were cured in ambient conditions, wrapped in plastic foil and tested after a rest period of 90 days after demolding. One more mortar subseries was cured the entire time in ambient conditions, and until the testing period samples were kept wrapped in a plastic foil. Ambient cured samples were tested after reaching the age of 90 days after demolding time.

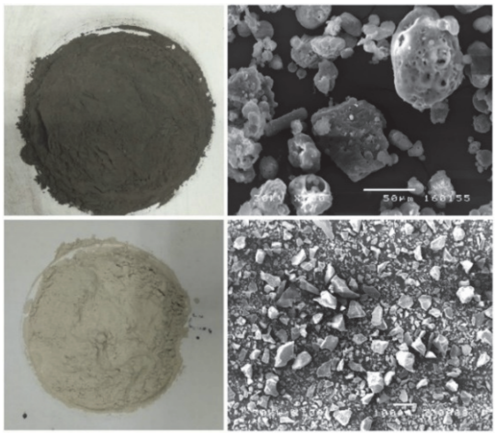

Figure 1 Photo (left) and SEM (right) display of used material: (up) fly ash, (down) ground granulated blast furnace slag

Table 3 Details of the mixtures

No	Mix.	FA / g	GGBFS / g	SP / %	Water / g	NaOH (10 M) / g	Na_2SiO_3 / g
1	0 S	450,00	-	2,0	20	56,16	303,23
2	12,5 S	393,75	56,25	1,5			
3	25 S	337,50	112,50	1,4			
4	37,5 S	281,25	168,75	1,2			
5	50 S	225,00	225,00	1,0			
6	62,5 S	168,75	281,25	0,8			
7	75 S	112,50	337,50	1,5			
8	87,5 S	56,25	393,75	1,2			
9	100 S	-	450,00	1,0			

Sodium hydroxide (SH) and sodium silicate (SS) manufactured by the local produces were used as alkali solutions. The SH was prepared by dissolving NaOH flakes (purity of 98%) in water to 10 m solution 24 hours prior to mixing. The SS activator was of the following characteristics: module (Ms = SiO_2/Na_2O) 2,2; content SiO_2 = 26.70%, Na_2O = 13.30% and H_2O = 60%). Liquids SS and SH were mixed in a mass ratio 100:18.52 (i.e. $Na_2SiO_3/NaOH$ = 5,40). Such ratio caused the creation of a single activator with a content of 10% Na_2O in respect to the mass of the solid binder (10% of 450 g, i.e. 45 g). This decreased the module of MS (SiO_2/Na_2O) in SS to the value of 1.5. Alkali solutions were mixed 30 minutes prior to the use. Such ratio of the liquid and solid phases was used in making of all geopolymer mixtures. Standard tap water was used during the mortar production in all mixtures.

The aggregate used was the river sand from the South Morava river (Serbia) with a maximum grain size of 2 mm. Binder (FA + GGBFS) to sand ratio 1:3 was the same in all mixtures. Details of mixtures are provided in Tab. 3.

3.3 Methods of Examinations

3.3.1 Experimental Examinations

Testing flexural and compressive strength of geopolymer mortar was performed according to the SRPS EN 196-1:2017 [36] standard at the sample age of 90 days. Flexural strength was tested on three prism samples having dimensions 40 × 40 × 160 mm, while the compressive strength was tested on the halves of mortar prisms which were previously tested to flexural strength.

3.3.2 Statistical Examinations

Gaussian process regression (GRP) the primary goal of this research is to develop a prediction model of compressive strength of geopolymer mortars. The required data was collected from the experimental laboratory testing of 45 series of geopolymer mortar. The obtained input-target values were then used to train the regression models. The input data includes curing temperature, percentage-mass content of FA and GGBFS, while the target value is compressive strength. The 80% of data was randomly taken for training and model validation, while the 20% of data was used for testing. The validation is done using 5 fold cross validation resampling procedure. The training data set was split into 5 randomly chosen subsets (or folds) of roughly equal size. One of these subsets is used for validation of the model trained using the rest of the subsets. This process is repeated 5 times so that each subset is used exactly once for validation.

Table 4 The kernel functions [31]

Name of kernel function	Equation
Squared Exponential Kernel	$k\left(x_i, x_j \mid \theta\right) = \sigma_f^2 \exp\left[\dfrac{-\left(x_i - x_j\right)^T \left(x_i - x_j\right)}{2\sigma_f^2}\right]$
Exponential Kernel	$k\left(x_i, x_j \mid \theta\right) = \sigma_f^2 \exp\left[\dfrac{-r}{\sigma_l}\right]$, $r = \sqrt{\left(x_i - x_j\right)^T \left(x_i - x_j\right)}$
Matern 3/2	$k\left(x_i, x_j \mid \theta\right) = \sigma_f^2 \left(1 + \dfrac{\sqrt{3}r}{\sigma_l} + \dfrac{3r^2}{3\sigma_l^2}\right) \exp\left(-\dfrac{\sqrt{3}r}{\sigma_l}\right)$, $r = \sqrt{\left(x_i - x_j\right)^T \left(x_i - x_j\right)}$
Matern 5/2	$k\left(x_i, x_j \mid \theta\right) = \sigma_f^2 \left(1 + \dfrac{\sqrt{5}r}{\sigma_l} + \dfrac{5r^2}{3\sigma_l^2}\right) \exp\left(-\dfrac{\sqrt{5}r}{\sigma_l}\right)$, $r = \sqrt{\left(x_i - x_j\right)^T \left(x_i - x_j\right)}$
Rational Quadratic Kernel	$k\left(x_i, x_j \mid \theta\right) = \sigma_f^2 \left(1 + \dfrac{r^2}{3\alpha\sigma_l^2}\right)$, $r = \sqrt{\left(x_i - x_j\right)^T \left(x_i - x_j\right)}$, α is a positive-valued scale-mixture parameter

As mentioned earlier, GRP requires kernel function. So, to find a model which best fits our data, regression models with different kernels for predicting mechanical characteristics were tested. Used kernel functions are presented in Tab. 4.

To obtain the best performance of each model, the Bayesian optimization was used for hyperparameter optimization. The performances of the proposed models were assessed for training and test data separately. The training set was used to fit and estimate the prediction error for the model selection (validation), while the test set was used to assess the generalization error i.e., how accurately the model can predict outcome values for previously unseen data.

The reliability and accuracy of the created models are evaluated via the *R*-squared, root mean square error (*RMSE*) and mean absolute error (*MAE*). Basically, a higher level of R^2 is an indicator of better accuracy of the model, while lower *RMSE* and *MAE* indicate lower deviations between measured and predicted values [37].

4 RESULTS AND DISCUSSION

The flexural strength test results of the geopolymer mortar mixtures are shown in Fig. 2. Each of the presented values is the average of three measurements of flexural strength at the age of 90 days. The highest value of flexural strength was measured on samples mixture named "0 S" and on the samples cured at ambient temperature it is 9,1 MPa. A slightly lower compressive strength was measured on the samples of geopolymer mortar of the same composition and equivalent age which, until the time of the test, were cured at the increased temperature conditions, ranging between 65 °C and 95 °C. Flexural strength of these mixtures ranged between 6,8 and 8,8 MPa. Flexural strength of geopolymer mortars made with GGBFS as only binder was lower than the mortars made with FA only.

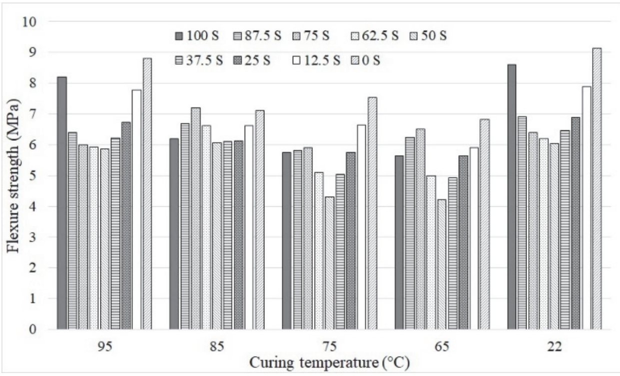

Figure 2 Flexural strength of geopolymer mortar cured at different curing temperature

In all the tested curing regimes, the lowest value of flexural strength had the samples marked as "50 S". The flexural strength which was measured on the samples of the mentioned series ranged between 4,2 and 6,1 MPa. Similar test results were obtained by Puertas et al. [38]. According to these authors, due to the replacement of FA with GGBFS to the percentage-mass content of 50% the flexural strength of mortar decreases. As the percentage-mass content of GGBFS becomes predominant in a binder, in relation to FA, the strength increases, while at 100% of GGBFS it reaches and surpasses the strength of the mixture made only with FA as a binder.

The compressive strength test results of the geopolymer mortar mixtures are shown in Fig. 3. Each value presented is the average of six measurements.

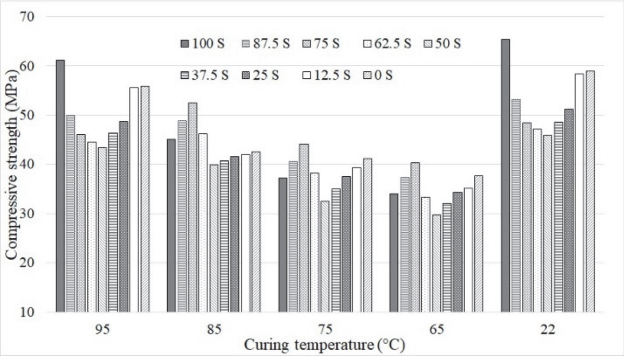

Figure 3 Compressive strength of geopolymer mortar cured at different curing temperature

As with flexural strength, the highest values of compressive strength were measured on samples that were cured in ambient conditions. The strength of samples cured at ambient temperature was 2% to 47% higher than the strength of samples cured at elevated temperature. Yet, the trend of strength increase is noticeable due to the increase of the curing temperature from 65 °C to 75 °C, 85 °C and 95 °C. Compressive strength of the mentioned samples ranges between 29,72 MPa (mixture "20 S" cured on 65 °C) and 61,12 MPa (mixture "100 S" cured on 95 °C). As in the case of flexural strength, compressive strength of the "50 S" mixture was the lowest at all curing conditions, while it was the highest for the "100 S" mixture. At an ambient curing regime, the compressive strength of the mentioned mixture is the highest, and it amounts to 65,35 MPa. The obtained test results are partly in agreement with the test results of other authors [38] who concluded that the compressive strength changes depend on the percentage-mass content of slag in the mixture which is a direct consequence of the created phases. Namely, due to the hardening of the mortar made only with FA as a binder, a N-A-S-H gel phase occurs as the dominant one [39], while in the mixtures made with GGBFS, due to the high content of CaO, a C-A-S-H gel phase occurs. However, the mortars made with a combination of FA and GGBFS are characterized by the occurrence of both gel phases, and the final system is the consequence of creation of C-A-S-H and N-A-S-H gels [40].

Gaussian process regression (GRP): In the proposed models, the amount of FA and GGBFS and curing temperature were considered as three input variables, while compressive strength was the output feature. Three different types of error indicators (R^2, *RMSE* and *MAE*) were used to indicate evaluation for the training and testing dataset. The training set was used to fit and estimate prediction error for model selection (validation), while test set was used to assess the generalization error i.e. how accurately the model can predict outcome values for previously unseen data.

The performances of the *GPR* models with different kernel function that corresponds to optimal values of kernel parameters are summarized in Tab. 5.

Relatively low values of *RMSE* and *MAE* as well as the high values of R^2 are indicators of the agreement of experimental and statistical data. According to the training results, the R^2 ranges between 0,82 and 0,86 and affects the high level of consistency of the training model. In general, R^2 presents a measure of how close the data is to the fitted regression line. The closer the values of R^2 are to 1, the better the proposed regression models are. The best performance was attained with the kernel function "Matern 3/2", and therefore, the results of GRP model with the "Matern 3/2" kernel function are reported. According to the training results *RMSE* value ranges between 3,2149 and 3,686 MPa, while in the test results it ranges between 4,51 and 4,82 MPa, what is acceptable.

Table 5 The kernel functions

Kernel function	Metric	R^2	*RMSE* / MPa	*MAE* / MPa
Squared Exponential Kernel	Training Results	0,82	3,6860	2,6574
	Test Results	0,61	4,8222	2,6799
Exponential Kernel	Training Results	0,82	3,6425	2,651
	Test Results	0,63	4,6474	3,1199
Matern 3/2	Training Results	0,86	3,2149	2,3352
	Test Results	0,67	4,4975	2,5047
Matern 5/2	Training Results	0,85	3,3046	2,4192
	Test Results	0,52	4,5094	2,4264
Rational Quadratic Kernel	Training Results	0,85	3,3023	2,4284
	Test Results	0,65	4,5166	2,4602

Fig. 4 illustrates the predicted response of our proposed model plotted against the measured compressive strength, while Fig. 5 shows the diagram of an estimation error. In Fig. 6 the regression results with a 95% confidence interval obtained on test dataset are shown.

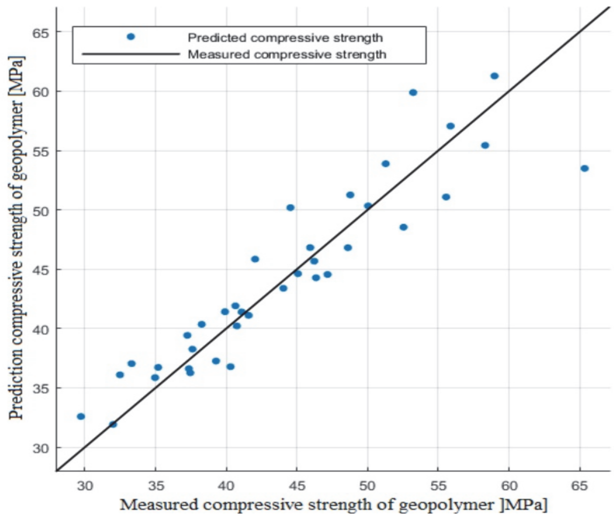

Figure 4 The predicted vs. true response of training data

Based on the obtained results it can be concluded that even with the low number of experimental data, the developed model can be used to predict the compressive strength of a geopolymer mixture made of different binders. Also, a good correlation between machine learning models and experimental results was obtained. The proposed models can be employed to build a standard geopolymer mortar mixture, and for designing the mix proportions of FA and GGNFS. We strongly believe that with a little more data, the GRP model will be able to make more accurate precision.

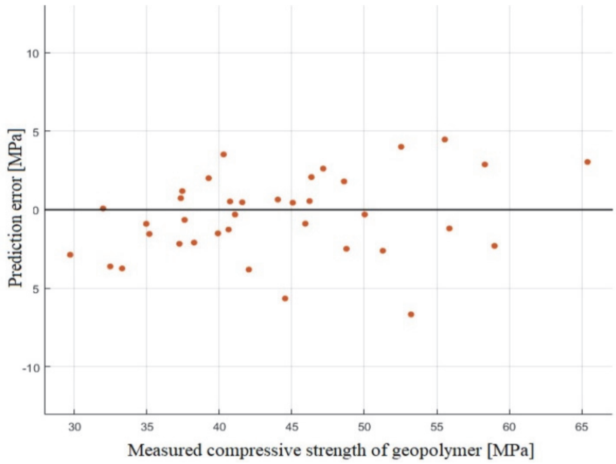

Figure 5 Absolute error of the predicted compressive strength of geopolymer

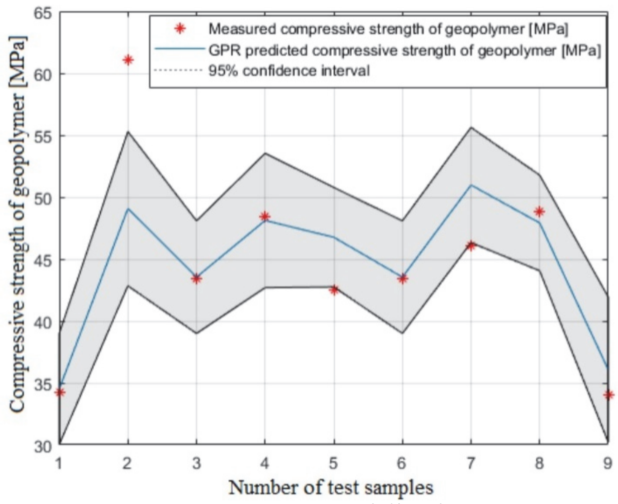

Figure 6 The regression results with a 95% confidence interval

5 CONCLUSIONS

This study focuses on modeling compressive strength values of geopolymer mortars by using the Gaussian robust regression method. A total of 45 datasets were used for the validation and training of the model. Experimental results were obtained by the laboratory testing of geopolymer mortars designed with GGBFS and FA as a binder. Mixtures were designed by replacing GGBFS in the amount of up to 100% of the total binder at the replacement step of 12,5%. Compressive strength was set as an output, while the other variable was the curing temperature between 22 °C and 95 °C.

According to the laboratory testing results, it can be concluded that the flexural and compressive strength change depending on the percentage-mass content of GGBFS in the binder and the implemented curing regime. The strengths of thermally activated samples of geopolymer mortars increase with increasing temperature. Maximum values are reached at an activation temperature of 95 °C, which is slightly less than the flexural and compressive strength of the samples cured for 90 days in ambient conditions. The increase in strength of ambient-cured samples of geopolymer mortars is slow, while thermally activated samples achieve between 90% and 95% of strength after 48 h, i.e. after the thermal activation.

According to the results of developed model, it can be concluded that the Gaussian robust regression can be used as a reliable regression method for prediction of compressive strength of FA and GGBFS based geopolymer mortars. In general, according to R^2 results, the capacity of the measured compressive strength of geopolymer reached up to 86%. So, according to the mentioned parameter it can be concluded that the created function is able to predict the compressive strength with a high level of accuracy and consistency. Future work should be focused on experimental work in order to form a larger dataset base which would lead to a creation of a better performing model.

6 REFERENCES

[1] Bijeljić, J. (2020). *Mogućnost primene industrijskih nusproizvoda u geopolimernim malterima i betonima na bazi elektrofilterskog pepela*. Faculty of civil engineering and architecture Niš.

[2] Bijeljić, J., Ristić, N., Grdić, Z., Ćurčić, G. T., & Đorđević, D. (2020). Durability properties of ladle slag geopolymer mortar based on fly ash.*Science of sintering*, *52*(2), 231-243. https://doi.org/10.2298/SOS2002231B

[3] Ivanović, M., Kljajević, Lj., Gulicovski, J., Petković, M., Castvan, I. J., Bučevac, D., & Nenadović, S. (2020). The effect of the concentration of alkaline activator and aging time on the structure of metakaolin based geopolymer.*Science of sintering*, *52*(2), 219-229. https://doi.org/10.2298/SOS2002219I

[4] Candamano, S., De Luca, P., Frontera, P., & Crea, F. (2017). Production of geopolymeric mortars containing forest biomass ash as partial replacement of metakaolin. *Environments*, *4*(4). https://doi.org/10.3390/environments4040074

[5] Torgal, F. P., Labrincha, J. A., Leonelli, C., Palomo, A., & Chindaprasirt, P. (2014). *Handbook of Alkali-Activated Cements, Mortars and Concretes*. Woodhead publishing series in civil and structural engineering.

[6] Jamstorp, E., Forsgren, J., Bredenberg, S., Engqvist, H., & Stromme, M. (2010). Mechanically strong geopolymers offer new possibilities in treatment of chronic pain. *Journal controlled release*, *146*(3). 370-377. https://doi.org/10.1016/j.jconrel.2010.05.029

[7] Adam, A. A. & Horianto, X. X. X. (2014). The effect of temperature and duration of curing on the strength of fly ash based geopolymer mortar. *Science Direct*, *95*, 410-414. https://doi.org/10.1016/j.proeng.2014.12.199

[8] Kumaravel, S. (2014). Development of various curing effect of nominal strength Geopolymer concrete. *Journal of Engineering Science and Technology Review*, *7*(1), 116-119. https://doi.org/10.25103/jestr.071.19

[9] Atis, C. D., Görür, E. B., Karahan, O., Bilim, C., Ilkentapar, S., & Luga, E. (2015). Very high strength (120 MPa) class F fly ash geopolymer mortar activated at different NaOH amount, heat curing temperature and heat curing duration. *Construction and building materials*, *96*, 673-678. https://doi.org/10.1016/j.conbuildmat.2015.08.089

[10] Bijeljić, J., Ristić, N., Grdić, Z., Ćurčić, G. T., Grdić, D., & Krstić, D. (2018). Effects of ground granulated blast furnace slag on physical-mechanical characteristics of geopolymer mortars based on fly ash. *14th International Scientific Conference (iNDiS), with Subconference "Eco build"*. University of Novi Sad, Faculty of tehnical sciences.

[11] Guo, X., Shi, H., & Dick, W. A. (2010). Compressive strength and microstructural characteristics of class C fly ash geopolymer". *Cement & concrete composites*, *32*, 142-147. https://doi.org/10.1016/j.cemconcomp.2009.11.003

[12] Rovnanik, P. (2010). Effect of curing temperature on the development of hard structure of metakaolin-based

geopolymer. *Construction and building materials*, *24*, 1176-1183. https://doi.org/10.1016/j.conbuildmat.2009.12.023

[13] Kaya, M., Uysal, M., Yilmaz, K., Karahan, O., & Atiş, C. D. (2020). Mechanical properties of class C and F fly ash geopolymer mortars. *Građevinar*, *72*(4), 297-309. https://doi.org/10.14256/JCE.2421.2018

[14] Mikoč, M., Bjelobrk, I., & Korajac, J. (2011). Alkali-activated fly ash concrete (Concrete without cement). *Technical Gazette*, *18*(1), 99-102.

[15] Pham, A., Hoang, N., & Nguyen, Q. (2016). Predicting compressive strength of high-performance concrete using metaheuristicoptimized least squares support vector regression. *Journal of Computing in Civil Engineering*, *30*(3). https://doi.org/10.1061/(ASCE)CP.1943-5487.0000506

[16] Nguyen, K. T., Nguyen, Q. D., Le, T. A., Shin, J., & Lee, K. (2020). Analyzing the compressive strength of green fly ash based geopolymer concrete using experiment and machine learning approaches. *Construction and building materials*, *247*, 118581. https://doi.org/10.1016/j.conbuildmat.2020.118581

[17] Dao, D. V., Ly, H. B., Trinh, S. H., Le, T. T., & Pham, B. T. (2019). Artificial intelligence approaches for prediction of compressive strength of geopolymer concrete. *Materials*, *12*(6), 983. https://doi.org/10.3390/ma12060983

[18] Dao, D. V., Trinh, S. H., Ly, H. B., & Pham, B. T. (2019). Prediction of compressive strength of geopolymer concrete using entirely steel slag aggregates: novel hybrid artificial intelligence approaches. *Applied science*, *9*(6), 1113. https://doi.org/10.3390/app9061113

[19] Cihan, M. T. (2021). Comparison of artificial intelligence methods for predicting compressive strength of concrete. *Građevinar*, *73*(6), 617-632. https://doi.org/10.14256/JCE.3066.2020

[20] Hoang, N. D., Pham, A. D., Nguyen, Q. L., & Pham, Q. N. (2016). Estimating compressive strength of high performance concrete with gaussian process regression model. *Advances in civil engineering*. https://doi.org/10.1155/2016/2861380

[21] Awoyera, P. O., Kirgiz, M. S., Viloria, A., & Gazabong, D. O. (2020). Estimating strength properties of geopolymer self-compacting concrete using machine learning techniques. *Journal of materials research and technology*, *9*(4), 9016-9028. https://doi.org/10.1016/j.jmrt.2020.06.008

[22] Bagheri, A., Nazari, A., & Sanjayan, J. (2019). The use of machine learning in boron-based geopolymers: Function approximation of compressive strength by ANN and GP. *Measurement*, *141*, 241-249. https://doi.org/10.1016/j.measurement.2019.03.001

[23] Panagiotopoulou, C., Tsivilis, S., & Kakali, G. (2015). Application of the Taguchi approach for the composition optimization of alkali activated fly ash binders. *Construction and building materials*, *91*, 17-22. https://doi.org/10.1016/j.conbuildmat.2015.05.005

[24] Lahoti, M., Narang, P., Tan, K. H., & Yang, E. H. (2017). Mix design factors and compressive strength prediction of metakaolin-based geopolymer. *Ceramics international*, *43*, 11433-11441. https://doi.org/10.1016/j.ceramint.2017.06.006

[25] Kamath, A., Hernández, R. A. V. R., Krems, V., Carrington, J. T., & Manzhos, S. (2018). Neural networks vs Gaussian process regression for representing potential energy surfaces: A comparative study of fit quality and vibrational spectrum accuracy. *The Journal of chemical physics*, *148*(24), 241702. https://doi.org/10.1063/1.5003074

[26] Mozumder, R. A., Laskar, A. I., & Hussain, M. (2017). Empirical approach for strength prediction of geopolymer stabilized clayey soil using support vector machines. *Construction and building materials*, *132*, 412-424. https://doi.org/10.1016/j.conbuildmat.2016.12.012

[27] Wang, J. (2020). An intuitive tutorial to gaussian processes regression.

[28] Fuentes, R., Gardner, P., Mineo, C., Rogers, T., Pierce, S., Worden, K., Dervilis, N., & Cross, E. (2020). Autonomous ultrasonic inspection using Bayesian optimisation and robust outliner analysis. *Computer science*. https://doi.org/10.1016/j.ymssp.2020.106897

[29] https://towardsdatascience.com/gaussian-process-regression-from-first-principles-833f4aa5f842

[30] Svensson, A. (2018). *Machine learning with state-space models, Gaussian processes and Monte Carlo methods*.

[31] Rasmussen, C. E. & Williams, C. K. I. (2016). *Gaussian processes for machine learning*, The MIT Press.

[32] SRPS B.C8.023:1997. Cement-Determination of bulk density.

[33] SRPS B.C1.018:2015. Non-metallic mineral raws 4-Pozzolanic materials - Constituents for cement production - Classification, technical conditions and test methods.

[34] SRPS EN 450-1. Fly ash for concrete - Part 1: Definition, specifications and conformity criteria.

[35] SRPS 15167-1:2010. Ground granulated blast furnace slag for use in concrete, mortar and grout - Part 1: Definitions, specifications and conformity criteria.

[36] SRPS EN 196-1:2017. Methods of testing cement - Part 1: Determination of strength.

[37] Chai, T. & Draxler, R. R. (2014). Root mean square error (*RMSE*) or mean absolute error (RMA)? Arguments against avoiding *RMSE* in literature. *Geosci. Model dev*, *7*, 1247-1250. https://doi.org/10.5194/gmd-7-1247-2014

[38] Puertas, F., Amat, T., Jimenez, A. F., & Vazquez, T. (2003). Mechanical and durable behaviour of alkaline cement mortars reinforced with polypropylene fibres. *Cement and concrete research*, 33(12), 2031-2036. https://doi.org/10.1016/S0008-8846(03)00222-9

[39] Palomo, A., Grutzek, M. W., & Blanc, M. T. (1999). Alkali-activated fly ashes. A cement for the future. *Cement and concrete research*, *29*, 1323-1329. https://doi.org/10.1016/S0008-8846(98)00243-9

[40] Puertas, F., Ramirez, S. M., Alonso, S., & Vazquez, T. (2000). Alkali activated fly ash/slag cements strength behaviour and hydratation productions. *Cement and concrete research*, *30*(10), 1625-1632. https://doi.org/10.1016/S0008-8846(00)00298-2

Contact information:

Nenad Ristić, PhD, associate prof.
(Corresponding author)
University of Nis,
Faculty of Civil Engineering and Architecture,
Aleksandra Medvedeva 14 street, 18000, Nis, Serbia
E-mail: nenad.ristic@gaf.ni.ac.rs

Emina Petrović, PhD, assistant prof.
University of Nis,
Faculty of Mechanical Engineering,
Aleksandra Medvedeva 14 street, 18000, Nis, Serbia
E-mail: emina.petrovic@masfak.ni.ac.rs

Jelena Bijeljić, PhD, senior lecturer
Academy of technical and educational vocational studies Niš,
Aleksandra Medvedeva 20 street, 18000, Nis, Serbia
E-mail: jelena.bijeljic@akademijanis.edu.rs

Miloš Simonović, PhD, teaching assistant
University of Nis,
Faculty of Mechanical Engineering,
Aleksandra Medvedeva 14 street, 18000, Nis, Serbia
E-mail: milos.simonovic@masfak.ni.ac.rs

Dušan Grdić, PhD, assistant prof.
University of Nis,
Faculty of Civil Engineering and Architecture,
Aleksandra Medvedeva 14 street, 18000, Nis, Serbia
E-mail: dusan.grdic@gaf.ni.ac.rs

Vlastimir Nikolić, PhD, Research Associate
University of Nis,
Faculty of Mechanical Engineering,
Aleksandra Medvedeva 14 street, 18000, Nis, Serbia
E-mail: vlastimir.nikolic@masfak.ni.ac.rs

Zoran Grdić, PhD, full prof.
University of Nis,
Faculty of Civil Engineering and Architecture,
Aleksandra Medvedeva 14 street, 18000, Nis, Serbia
E-mail: zoran.grdic@gaf.ni.ac.rs