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INTERACTION ANALYSIS AND MECHANICAL PREDICTION MODEL OF COAL GANGUE-BASED GEOPOLYMER

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This work analyses interaction factors affecting the preparation of a geopolymer from coal gangue and establishes an accurate mechanical prediction model to efficiently predict the flexural and compressive strength. Coal gangue is the main raw material, and NaOH and water glass are chosen as the activators to synthesise the geopolymer. First, response Surface Methodology (RSM) was applied to analyse the interaction impacts of the water glass modulus, liquid-to-solid ratio, sodium silicate/coal gangue ratio, and curing temperature on the mechanical properties. After that, a modified Support Vector Machine (SVM) and RSM were applied to establish a mechanical prediction model. The results reveal that there are two key interaction factors for the geopolymer properties. First, the water glass modulus and liquid-to-solid ratio could jointly affect the flexural strength. At the same time, the compressive strength is simultaneously influenced by the water glass modulus and curing temperature. Moreover, the analysis of the mechanical prediction models indicates that both the RSM and modified SVM could use little experimental data to predict the mechanical properties of geopolymer. However, the modified SVM has better prediction accuracy. Therefore, this study could efficiently predict the mechanical strength of a coal gangue-based geopolymer, conserve energy, and decrease the environmental pollution resulting from coal gangue.

INTRODUCTION

A geopolymer is an inorganic aluminosilicate material, which was firstly proposed by Davidovits in 1978 [1]. It has a three-dimensional framework comprised of $[AlO_4]$ and $[SiO_4]$ units [2]. Compared with ordinary Portland cement, a geopolymer exhibits several excellent performances with regards to its mechanical properties, acid corrosion resistance and thermal stability [3]. Based on the above advantages, it has been widely applied in the construction industry, in waste treatment, in emergency repairs and even in the solidification of radioactive waste [4]. Geopolymer were initially prepared by using metakaolin as the main raw material under the geopolymerisation of the activator [5]. After continuous development, the selection range of the raw materials for geopolymers has been expanded to include natural minerals, industrial waste, construction waste and agricultural residue which are abundant in aluminosilicates [6].

Coal gangue is a type of solid waste produced in the process of coal mining and washing [7]. The chemical composition of coal gangue mainly consists of Al_2O_3, SiO_2, Fe_2O_3 and CaO [8]. As the coal industry vigorously grew, a great deal of coal gangue waste was produced. On the one hand, the waste occupies too much land space for stacking, causing a serious waste of resources. On the other hand, due to the lack of proper management for the mining residue, toxic ions in the coal gangue could gradually spread in the environment, which can result in serious pollution [9, 10]. With the enhancement of environmental protection awareness, the comprehensive utilisation of coal gangue has attracted the attention of researchers [11–13]. However, the utilisation rate of coal gangue is still very low. Currently, there are few researchers who consider coal gangue to synthesise geopolymers [14–16].

Moreover, previous investigations indicate that the single variable method and orthogonal design method are usually adopted to study the effects of different factors on the geopolymer performance properties [17, 18]. Although these two methods could determine the effects of different factors on the geopolymer properties, the interactions among multiple factors on the flexural and compressive strength of a geopolymer should be addressed. Response Surface Methodology (RSM) can conveniently solve this problem. RSM is a comprehensive mathematical and statistical method, it can solve multivariant problems by reasonable experimental design and establish the relationship between the factors and the response values [19]. RSM was initially put forward by Box in the 1950s. Currently, it is generally used in the optimisation of the mixing proportions for concrete [20, 21]. However, RSM is seldom applied to analyse the interactions affecting the preparation of geopolymers.

Furthermore, as everyone knows, the flexural strength and compressive strength are two important parameters required to characterise the mechanical properties of cementitious materials. In the analysis of the flexural and compressive strength, most of the existing evaluation methods need to prepare a large number of specimens and use specific instruments to test their mechanical properties after a long period of curing. These assessment methods are accurate, but extremely time-consuming. Due to several complex relationships between the composition of the raw materials and the properties of cement-based materials, the prediction of mechanical properties has become a complicated multivariable and non-linear problem. The prediction by a conventional analysis and statistical method is not accurate enough for the flexural and compressive strength, it is also difficult to widely apply it in practice. A support vector machine (SVM) is a novel machine learning algorithm with prediction abilities, which was proposed by Sain and Vapnik [22]. SVM classifies data by supervised learning. Compared with traditional machine learning algorithms, SVM does not depend on a mathematical model of the system and has characteristics of self-learning and self-adjusting. It can produce good prediction results for various chaotic systems. Moreover, SVM uses different kernel functions to train models and give prediction results. The main kernel functions are linear, polynomial, and radial basis functions. Different models are built with different kernel functions, and their prediction accuracy is also different [23]. SVM has been successfully used to solve concrete related problems [24, 25], however, there are few reports on predicting the mechanical properties of geopolymers.

Based on the above analyses of the key interaction factors affecting the geopolymer synthesis from coal gangue, the present work aims to establish an accurate mechanical prediction model to efficiently predict the flexural and compressive strength. In this work, coal gangue was selected as the main raw material to prepare a coal gangue-based geopolymer, and RSM and SVM were introduced to study the influences of the water glass modulus, liquid-to-solid ratio, sodium silicate/coal gangue ratio, curing temperature and their interactions on the flexural strength and compressive strength. As a result, the impacts of the key factors and interactions of multiple factors were determined for the compressive strength and flexural strength of the coal gangue-based geopolymer. Moreover, in accordance with the mechanical properties testing and XRD and SEM analysis of the coal gangue-based geopolymer, a macro and micro analysis were carried out to optimise the mix design of the coal gangue-based geopolymer. In addition, the RSM and modified SVM were applied to establish a mechanical prediction model of the coal gangue-based geopolymer by using little experimental data. Therefore, the compressive strength and flexural strength of coal gangue-based geopolymer were predicted and analysed efficiently. This work provides a novel interaction analysis method and accurate mechanical prediction model for improving the synthesis of coal gangue-based geopolymers with outstanding mechanical performances. Furthermore, coal gangue was innovatively applied to prepare a geopolymer, which expands its application scope and decreases any solid waste pollution.

EXPERIMENTAL

Materials

The coal gangue was purchased from a local supplier in China. Since an alkaline excitation agent could not activate the raw coal gangue, it was necessary to break the interlayer structure of the coal gangue to obtain any pozzolanic activity after proper high-temperature calcination. First, the coal gangue was heated to 800 °C in a muffle furnace for 3 hours. Then grinding was conducted; the particle diameter of the treated coal gangue powder is about 44 μm, its density is 2.32 $g\cdot cm^{-3}$, its specific gravity is about 2.32 and its specific surface area is 396 $m^2\cdot kg^{-1}$. After the above steps, an alkaline activator could activate the calcined coal gangue to form a geopolymer. The coal gangue powders before and after calcination are presented in Figure 1.

A compound alkaline excitation agent was synthesised by using water glass and a sodium hydroxide solution in this work. The water glass was obtained from commercial suppliers. The water glass modulus is 3.3, and the full chemical composition of the water glass includes sodium silicate (Na_2SiO_3) and water. The solid content of the water glass is 38.7 wt. %. Sodium hydroxide is an analytical reagent grade with a purity of 99.31 %, purchased from a commercial company.

Experiment design

RSM is a low-cost and efficient experimental design approach, which could significantly decrease the time of the experiment. The Box-Behnken design method of Design-Expert 11 software was applied to

a) coal gangue powder b) calcined coal gangue powder

Figure 1. Coal gangue powder before and after calcination.

design the experiment, the effects of the modulus of water glass (A), sodium silicate/coal gangue ratio (B), liquid-to-solid ratio (C) and curing temperature (D) on the compressive strength (Y1) and flexural strength (Y2) were studied. Table 1 lists the factors and levels that need to be considered in the experiment.

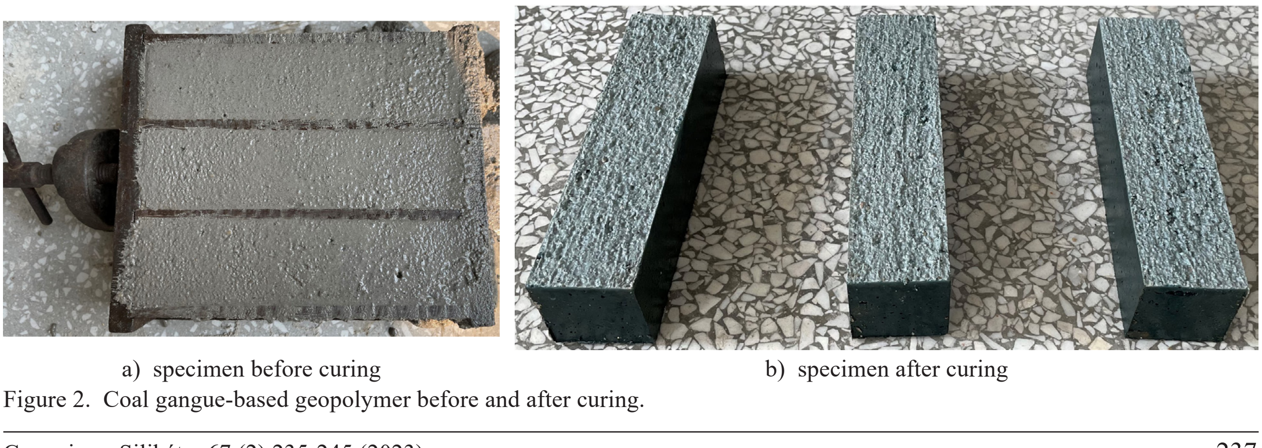
Table 1. Factors and levels of the RSM.

Factor	Code	Level of code		
		-1	0	1
Modulus of water glass	A	1.00	1.20	1.40
Sodium silicate/ /coal gangue ratio	B	0.40	0.42	0.44
Liquid-to-solid ratio	C	0.85	0.90	0.95
Curing temperature	D	30 °C	50 °C	70 °C

The synthesis, testing and characterisation of the coal gangue-based geopolymer

An alkali activator was prepared first based on the above experiment design and previous research [26]. To obtain water glass with a modulus of 1.0, 1.2, and 1.4, 25.44 g, 19.41 g, and 15.11 g, NaOH flakes were added to 100 g of water glass. In terms of the above proportion, the NaOH flakes and water glass were separately weighed. After that, the NaOH flakes were added to the water glass solution slowly with continuous mixing until the NaOH flakes were dissolved thoroughly. The prepared alkali activator was kept at ambient temperature for one day prior to use.

Secondly, the calcined coal gangue powder was selected as a raw material to prepare the geopolymer by an alkali activation reaction. The powder, obtained from the prepared alkali activator solution, and the deionised water were weighed according to the sodium silicate/coal gangue ratio and liquid-to-solid ratio requirement and stirred thoroughly for 5 minutes in a mechanical stirrer. Afterward, the prepared slurries were transferred to a 40 mm × 40 mm × 160 mm mould. In order to eliminate entrapped air in slurries, all the slurries were vibrated for 180 seconds. Finally, the coal gangue-based geopolymer specimens were divided into three groups; these different groups were cured at different temperature (30 °C, 50 °C and 70 °C). After 24 hours, all the specimens were removed from the moulds and cured at an ambient temperature for 28 days. Figure 2 illustrate that coal gangue-based geopolymer before and after curing.



a) specimen before curing b) specimen after curing

Figure 2. Coal gangue-based geopolymer before and after curing.

A NYL-300 electronic universal tester and a TYE-10C flexural tester were applied to carry out the compressive test and flexural test on the coal gangue-based geopolymer samples with a curing age of 28 days. All the test results were based on the average of six geopolymer specimens.

Scanning electron microscopy (ZEISS-SUPRA40) was conducted to observe the microstructure of the fractured coal gangue-based geopolymer under an accelerating voltage of 20 kV.

A specific surface area tester (Micromeritics TriStar II Plus) was applied to measure the pore size, porosity, and specific surface area of the coal gangue-based geopolymer.

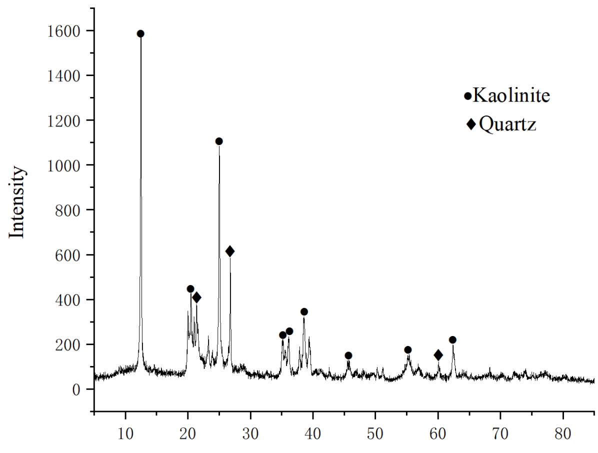
An X-ray fluorescence (XRF) spectrometer (Axios PW4400) was applied to study the key chemical composition of the coal gangue and calcined coal gangue. The results are listed in Table 2.

Table 2. Chemical composition of the coal gangue and calcined coal gangue.

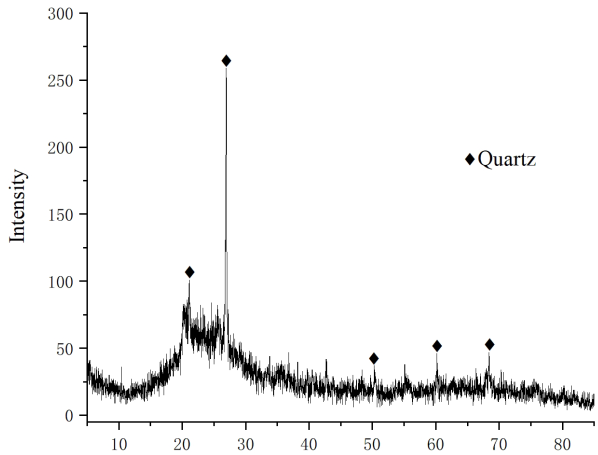
Composition	SiO_2	Al_2O_3	Na_2O	MgO	P_2O_5	K_2O	SO_3	TiO_2	CaO	Fe_2O_3
Gangue (%)	54.978	40.457	0.088	0.137	0.061	0.921	0.331	1.455	0.473	1.097
Calcined gangue [26] (%)	53.415	42.292	0.163	0.214	0.049	0.893	0.229	1.328	0.343	1.067

The results of the XRF in Table 2 indicate that the chemical composition of the coal gangue only change a little before and after calcination. Its main components, SiO_2 and Al_2O_3, are silicon and aluminium sources for the geopolymer, with the total weight of SiO_2 and Al_2O_3 being over 95 %.

X-ray diffraction (XRD) (Bruker D8 Advance) was applied to implement the mineralogical characterisation for the original coal gangue, calcined coal gangue, and coal gangue-based geopolymer specimens. Jade 6.5 software was used to perform the qualitative analysis of the crystalline and amorphous phases by comparing the diffraction patterns to the International Centre for Diffraction Data PDF2-2004 database. The XRD patterns of both the natural coal gangue and calcined coal gangue powder are presented in Figure 3.



a) natural coal gangue



b) calcined coal gangue

Figure 3. XRD patterns of the natural coal gangue and calcined coal gangue [26].

Establishment of the mechanical prediction model

In this paper, the Response Surface Methodology (RSM) and an improved Support Vector Machine (SVM) were used to establish the flexural and compressive strength models of the coal gangue-based geopolymer with a 28-day curing age. The models established by two different methods were applied to respectively predict the compressive and flexural strength of the coal gangue-based geopolymer.

RSM utilised a second order polynomial to fit the experimental data. The quality of model was assessed by a correlation coefficient R^2 and the mean square error M. The RSM model is as follows [21].

$$y=\beta_0+\sum_{i=1}^{m}\beta_i x_i+\sum_{i<j}^{m}\beta_{ij}x_i x_j+\sum_{i=1}^{m}\beta_{ii}x_i^2+\varepsilon$$

Where y is response; x_i and x_j are the factors; β_0, β_i, β_{ij} and β_{ii} represent the regression coefficients; ε represents the random error of the equation.

The flexural strength and compressive strength of the coal gangue-based geopolymer are not only closely related to the mix ratio, but also depend on the curing temperature. Therefore, it is a complicated and non-linear function relationship. In order to predict the flexural strength and compressive strength of the coal gangue-based geopolymer by the improved SVM model, it was necessary to determine the input and output variables of the SVM, and then the data of the learning sample were divided into a training set and a test set. SVM established the function relationship between the input and output variables by training and simulating the data. Finally, a prediction model of the geopolymer strength can be obtained. Four factors affecting the strength of the coal gangue-based geopolymer for 28 days were considered in this study: the water glass modulus, sodium silicate/coal gangue ratio, liquid-to-solid ratio and curing temperature. These factors were selected as the input variables of the modified SVM, and the results of the 28-day flexural strength and compressive strength were taken as the two output nodes of the modified SVM network.

Moreover, the selection of the kernel function is a core issue in the study of the SVM theory, and its choice significantly impacts the SVM model. Choosing different kernel functions could result in various machine-learning algorithms. Currently, there is no uniform and effective method to efficiently choose suitable kernel functions for the SVM. Previous experimental results showed that the radial basis function is an appropriate kernel function for the SVM model of coal gangue-based geopolymers.

The data set was obtained from the experimental design by Response Surface Methodology. It can be used to predict the mechanical performances of coal gangue-based geopolymers. The experimental data were divided into two categories, one was a training set and the other was a test set. The data in the training set were used to build the mechanical prediction model, and the data in the test set were applied to validate and modify the model.

RESULTS AND DISCUSSION

Interaction analysis

In this study, all the experiments use the RSM design. In order to decrease the experimental error, five central points are set. The experimental results are listed in Table 3.

Design Expert 11 was used to carried out the regression analysis to obtain the experiment results. The

Table 3. Design of the experiment and experimental results.

Experiment Number	Factor				Flexural Strength (MPa)	Compressive strength (MPa)
	Modulus of water glass	Sodium silicate/ /coal gangue ratio	Liquid-to-solid ratio	Curing temperature		
1	1	0	1	0	4.3	47.4
2	1	1	0	0	6.1	58.6
3	0	0	0	0	7.4	61.7
4	-1	-1	0	0	5.7	57.3
5	0	0	1	1	5.2	52.7
6	-1	0	-1	0	7.9	64.1
7	0	1	0	-1	7.3	60.2
8	0	0	1	-1	4.8	50.6
9	0	0	-1	1	8.3	65.9
10	-1	0	0	1	7.2	59.5
11	-1	0	1	0	4.4	50.9
12	0	1	0	1	7.5	60.8
13	0	0	-1	-1	8.0	65.4
14	1	0	0	-1	5.5	57.4
15	0	0	0	0	7.4	61.7
16	0	-1	-1	0	7.8	63.9
17	0	1	1	0	5.3	53.7
18	0	0	0	0	7.4	61.7
19	0	0	0	0	7.4	61.7
20	0	-1	0	1	7.0	60.6
21	0	0	0	0	7.4	61.7
22	0	1	-1	0	8.1	65.6
23	0	-1	1	0	4.7	51.3
24	-1	1	0	0	6.7	57.8
25	1	0	-1	0	6.9	62.5
26	-1	0	0	-1	6.5	56.6
27	0	-1	0	-1	6.3	59.2
28	1	-1	0	0	5.8	56.7
29	1	0	0	1	6.0	57.0

results are presented in Table 4. The F value reveals the extent to which the response is affected by the factors. The larger the value, the greater impact on the response. The P value indicates the significance level of the factor. With a decreasing P value, the significance level of the factors gradually increases. When the P value is less than 0.05, it is demonstrated that the factor is significant. If the P value is smaller than 0.0001, it means the factor is extremely significant [26].

Table 4 shows an extensive sequence of each factor on the compressive strength of the geopolymer. The highest level of influence degree is caused by the liquid-to-solid ratio. The sodium silicate/coal gangue ratio and the curing temperature, respectively, are the second level and third level of significance. The water glass modulus attributes the lowest influence on the 28-d compressive strength.

Table 4. Regression analysis for the flexural and compressive strength of the geopolymer.

Factor	Flexural strength (28d)		Compressive strength (28d)	
	F value	P value	F value	P value
A- Modulus of water glass	31.64	< 0.0001	7.27	0.0174
B- Sodium silicate/coal gangue ratio	29.99	< 0.0001	9.89	0.0072
C- Liquid-to-solid ratio	733.72	< 0.0001	1089.53	< 0.0001
D- Curing temperature	17.18	0.0010	8.41	0.0116
AB	3.22	0.0943	0.9813	0.3387
AC	5.32	0.0368	1.81	0.2002
AD	0.2629	0.6161	5.45	0.0349
BC	0.5915	0.4546	0.2453	0.6281
BD	1.64	0.2207	0.3204	0.5803
CD	0.0657	0.8014	1.28	0.2766
A^2	157.99	< 0.0001	139.68	< 0.0001
B^2	15.35	0.0015	8.14	0.0128
C^2	66.62	< 0.0001	66.01	< 0.0001
D^2	3.22	0.0942	7.64	0.0152

Table 4 shows that the water glass modulus, sodium silicate/coal gangue ratio, and liquid-to-solid ratio have tremendous effects on the flexural strength of the 28-d geopolymer specimens ($P < 0.0001$), and the curing temperature has a significant impact ($P < 0.05$) on the flexural strength. According to the F value, the order of influence degree for each factor on the flexural strength of the coal gangue-based geopolymer is shown below: liquid-to-solid ratio > water glass modulus > sodium silicate/coal gangue ratio > curing temperature. Moreover, there is an interaction between the water glass modulus and liquid-to-solid ratio for the flexural strength ($P < 0.05$). For the 28-day compressive strength of the sample, the liquid-to-solid ratio has highly significant effects on the compressive strength ($P < 0.0001$). Moreover, Table 4 indicates that the water glass modulus, sodium silicate/coal gangue ratio, and curing temperature significantly impact the preparation of the geopolymer ($P < 0.05$). Furthermore, the interaction between the water glass modulus and curing temperature also has a significant impact on the compressive strength of the sample. Furthermore, the F value in

Pore structure analysis

Due to the fact that the mechanical properties of the coal gangue-based geopolymer highly depend on their pore size, specific surface area and porosity, thus, in this work, both the coal gangue-based geopolymer with the lowest and the highest mechanical strength had a pore structure analysis conducted. The pore structure parameters are listed in Table 5.

According to Table 5, it can be found that average pore size of both types of geopolymers are less than 50 nm, therefore, the pores in the coal gangue-based geopolymer are mainly mesoporous. The average pore diameter of the coal gangue-based geopolymer with the lowest mechanical strength is about 28.5 nm, while the coal gangue-based geopolymer with the highest mechanical strength has a smaller pore size, which is 24.7 nm. Both the specific surface area and porosity have a similar trend. This indicates that the pore structure greatly affects the mechanical strength of the coal gangue-based geopolymer, a smaller pore size, specific surface area and porosity could result in a higher mechanical strength.

Table 5. Pore structure parameters of the coal gangue-based geopolymer.

Coal gangue-based geopolymer	Average pore diameter (nm)	Specific surface area ($m^2 \cdot g^{-1}$)	Porosity (%)
The lowest mechanical strength	28.5	19.26	22.14
The highest mechanical strength	24.7	17.30	16.52

Crystalline phases and microstructure analysis

The coal gangue-based geopolymer specimen with best performance was selected in order to carry out a mineralogical analysis by XRD. Figure 4 shows the results.

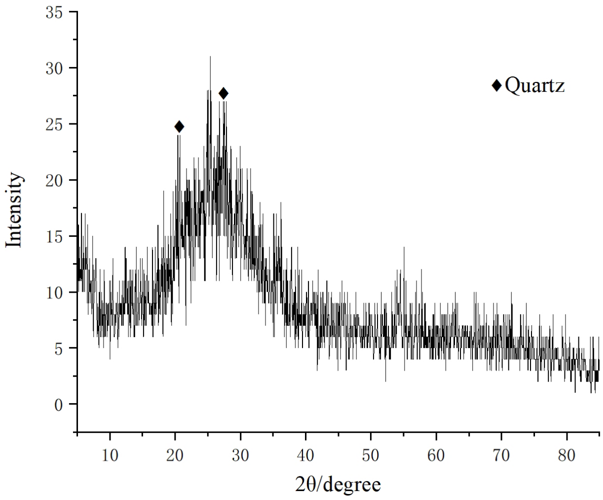
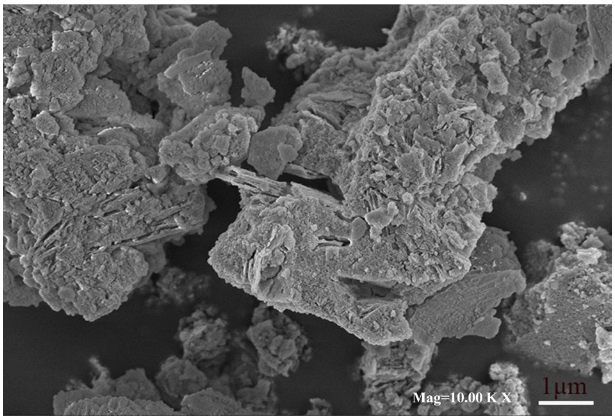


Figure 4. XRD pattern of the coal gangue-based geopolymer at 28 days of curing [27].

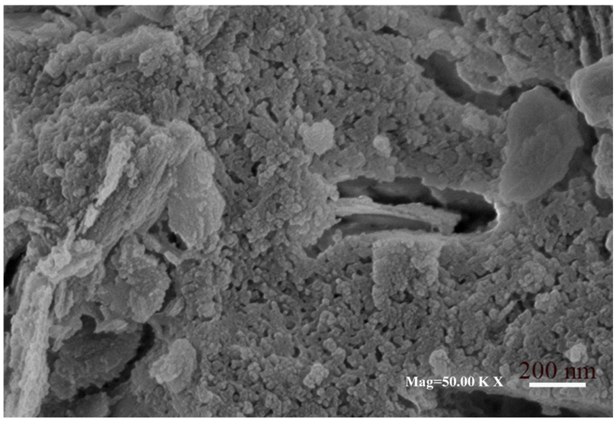
Figure 4 demonstrates that there is a broad diffraction peak between 10° to 40° (2θ) in the XRD pattern. It can indicate that amorphous substances are dominant components in the geopolymer. Compared with the XRD pattern of the calcined gangue powder, the reflection peak of the geopolymer shifts towards a high theta angle value. It means that there are new amorphous substances produced by the geopolymerisation. The new amorphous products are mainly aluminosilicate gels [27]. Moreover, a small amount of diffraction peaks of quartz can be found, which is due to the unreacted residue in the raw materials.

The coal gangue-based geopolymer with the lowest flexural strength and compressive strength was selected for the microstructure analysis by SEM. Meanwhile, a similar analysis was implemented for the sample with the highest strength. All the results are shown in Figure 5.

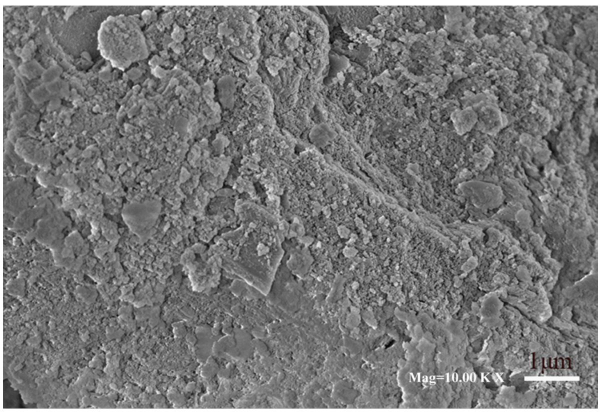
Figure 5 demonstrates that the internal morphology of the geopolymer is a highly dense microstructure, formed by the cementation of sodium aluminosilicate hydrate gels and unreacted coal gangue particles. Compared to the morphology of the specimens with the lowest and highest strength, it is found that there are some pores on the surface of low-strength geopolymer, but not on the surface of geopolymer with high



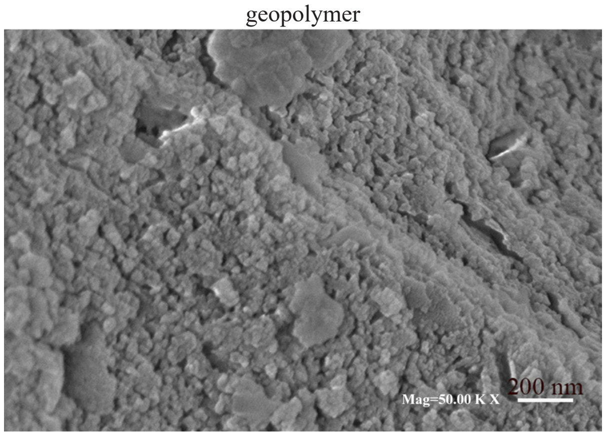
a) low magnification SEM for the lowest strength geopolymer



b) high magnification SEM for the lowest strength geopolymer



c) Low magnification SEM for the highest strength geopolymer



d) High magnification SEM for the highest strength geopolymer

Figure 5. SEM for the morphology and microstructure analysis of the geopolymer.

mechanical performance. It indicates that the structure of the high-strength geopolymer sample are more compact than the low-strength one. The mix proportion and curing temperature of the high strength geopolymer increase the reaction degree of the calcined coal gangue and promote the geopolymerisation. With the increase in the geopolymerisation reaction, the massive coal gangue powders gradually dissolve, depolymerise and reorganise, and then a more amorphous geopolymer gel will be produced. The hydrate gel is a key factor in the development of the strength. Thus, the more geopolymer gels produced by the geopolymerisation reaction can make the sample's internal structure more compact and, therefore, the geopolymer has higher strength. The analysis results of the scanning electron microscopy are consistent with the pore structure analysis.

Comparison and analysis of the mechanical prediction models

RSM prediction model

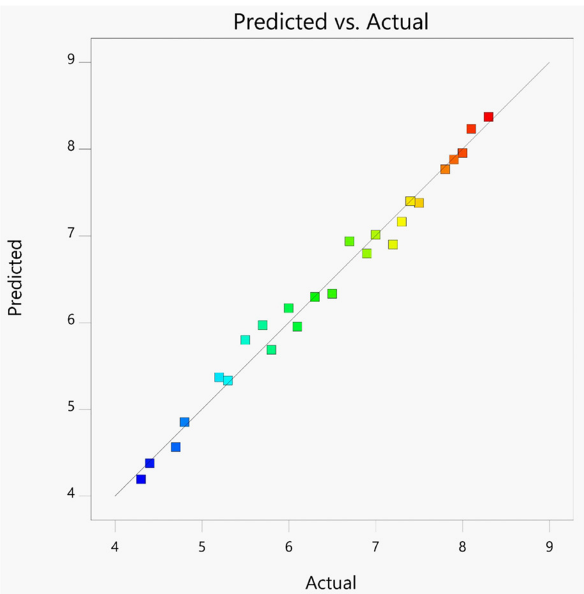
RSM was applied to fit the experimental data and the flexural and compressive strength model of the coal gangue-based geopolymer were obtained. Table 6 lists the results.

The R^2 values of the flexural and compressive strength models are 0.9865 and 0.9894 in Table 6, respectively. The R^2 value of the two models approaches 1. It indicates that these two models have high reliability and a slight deviation. Moreover, Table 6 shows that the P value of the flexural and compressive strength models is smaller than 0.0001, which shows the significance of the two established models [26].

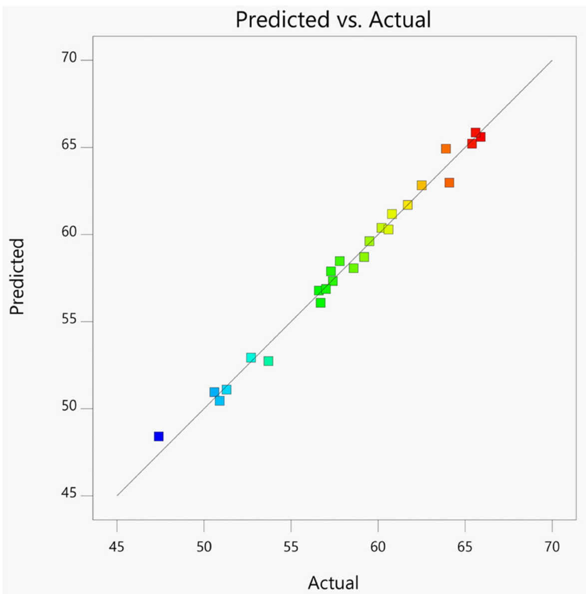
The plots of the predicted and experimental values of the flexural strength and compressive strength are presented in Figure 6. It can be used to assess the prediction quality of the RSM model. The colour points

Table 6. Flexural and compressive strength model of the RSM for the geopolymer.

Model	Equation	R^2	Adjusted R^2	F value	P value
Flexural strength	$+ 7.40 - 0.3167 * A + 0.3083 * B - 1.53 * C + 0.2333 * D - 0.1750 * AB + 0.2250 * AC - 0.0500 * AD + 0.0750 * BC - 0.1250 * BD + 0.0250 * CD - 0.9625 * A^2 - 0.3000 * B^2 - 0.6250 * C^2 - 0.1375 * D^2$	0.9865	0.9729	72.82	< 0.0001
Compressive strength	$+ 61.70 - 0.5500 * A + 0.6417 * B - 6.73 * C + 0.5917 * D + 0.3500 * AB - 0.4750 * AC - 0.8250 * AD + 0.1750 * BC - 0.2000 * BD + 0.4000 * CD - 3.28 * A^2 - 0.7917 * B^2 - 2.25 * C^2 - 0.7667 * D^2$	0.9894	0.9787	92.94	< 0.0001



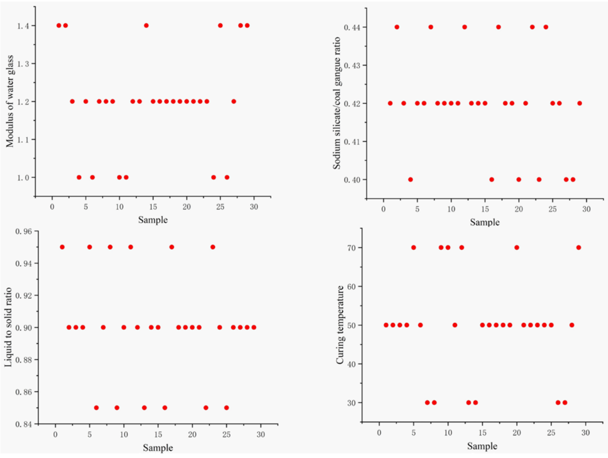
a) distribution of the flexural strength



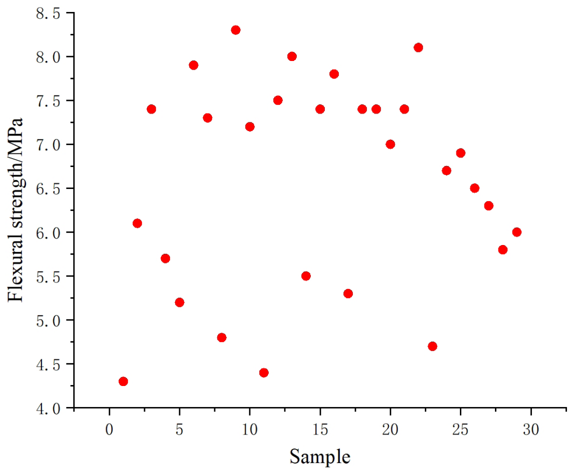
b) distribution of the compressive strength

Figure 6. Distribution of the predicted and experimental values for the flexural and compressive strength by RSM.

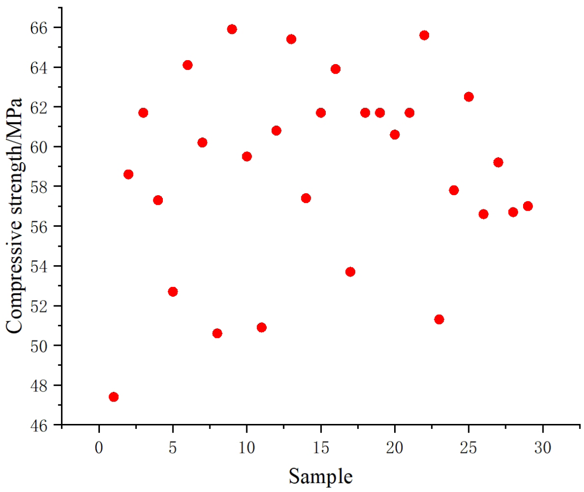
represent the value of the flexural strength and the compressive strength. When each colour point in the figure is distributed around a straight line, it indicates that the model's prediction accuracy is higher. Figure 6a and 6b demonstrate that RSM's flexural and compressive strength models exhibit good prediction quality.



a) distribution of the input data for the SVM prediction model



b) distribution of the output data for the flexural strength



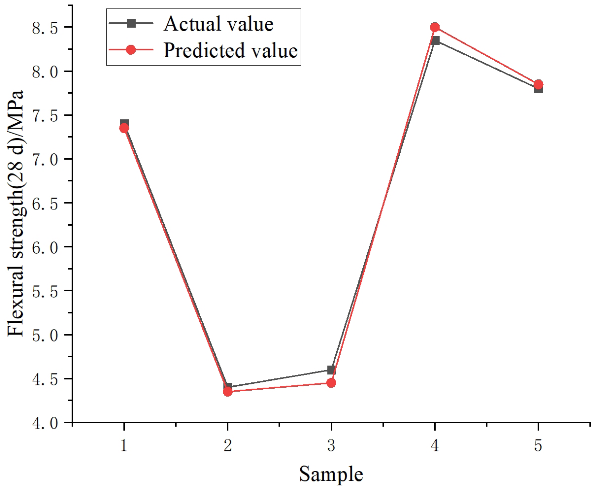
c) distribution of the output data for the compressive strength

Figure 7. Distributions of the input and output data for the SVM model.

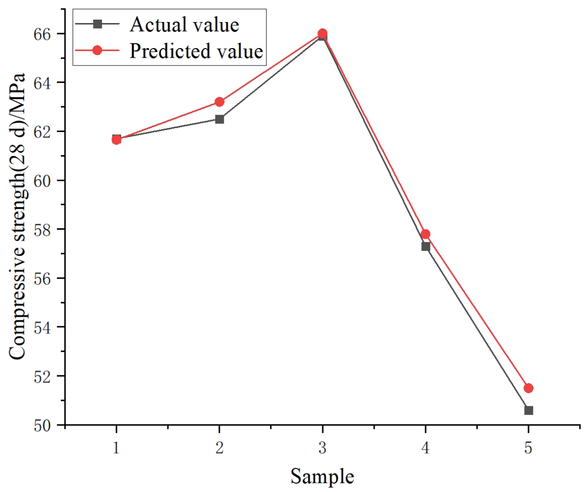
Modified SVM prediction model

SVM was applied to build a flexural and compressive strength model of the geopolymer. Twenty groups of experimental data were randomly selected as training sets, and the remaining five groups were used as the test sets. Four factors were taken as the input parameters of the SVM. They are the water glass modulus, sodium silicate/coal gangue ratio, liquid-to-solid ratio and curing temperature. The flexural and compressive strength test data were chosen as the output responses, and the radial basis function (RBF) was selected as the kernel function of the SVM. The distributions of the four input and two output data are shown in Figure 7.

Moreover, the prediction accuracy of the model not only depends on the input and output data, but also relies on the optimisation of the SVM parameters. Therefore, a genetic algorithm was applied to improve the original SVM model, the genetic algorithm could automatically look for the appropriate SVM parameters in this work. Figure 8 shows the modified SVM model's prediction results of the flexural strength and compressive strength.



a) distribution of the input data for the SVM prediction model



b) distribution of the output data for the flexural strength

Figure 8. Predicted and experimental value of the flexural strength and compressive strength.

It was found that predicted values are in good agreement with the experimental data. The standard deviation R^2 for the flexural and compressive strength is 0.99118 and 0.99414, respectively. It indicates that the prediction error of the model is negligible and the construction of the modified SVM prediction models are successful. Comparing the RSM models, it can be found that both methods fit the experimental data efficiently, but the flexural and compressive strength models built by the modified SVM have a better data fitting ability and prediction accuracy than the model built by the RSM. The modified SVM that was applied to build the complex mechanical prediction model has the advantages of simple and convenient process and a high fitting degree.

CONCLUSIONS

In this paper, RSM and a modified SVM were applied to study the interactions affecting the preparation of a geopolymer from coal gangue, and establish a mechanical prediction model to predict the flexural and compressive strength efficiently. This study could optimise the preparation of the coal gangue-based geopolymer, expand the application scope of coal gangue and decrease any solid waste pollution. The main conclusions are as follows:

(1) The results of the RSM analysis reveal that the flexural strength and compressive strength are not only affected by single factor, but also the interaction of the water glass modulus and the liquid-to-solid ratio, as well as the interaction of the water glass modulus and the curing temperature, which separately affect the flexural strength and compressive strength.

(2) The crystalline phase and microstructure analysis indicate that an amorphous network structure was formed by the depolymerisation and condensation of [SiO_4] and [AlO_4] tetrahedrons. It can bind with the unreacted particles of the calcined coal gangue to form a dense hydrate gel structure, which results in the higher flexural and compressive strength of the samples.

(3) The comparison of the different mechanical prediction models demonstrates that when the amount of experimental data is relatively small, both the RSM and modified SVM could predict the mechanical properties of the geopolymer accurately. However, the modified SVM has a higher prediction accuracy.

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