

Şinasi Bingöl^{1*}, İlker Günay²

^{1*} Tokat Gaziosmanpaşa University, Faculty of Engineering and Architecture, Civil Engineering Department, Türkiye

² Tokat Gaziosmanpaşa University, Faculty of Engineering and Architecture, Computer Engineering Department, Türkiye

* sinasi.bingol@gop.edu.tr

WASTE-DERIVED GEOPOLYMER MORTARS FROM INDUSTRIAL SLAGS: MODELING EARLY-AGE COMPRESSIVE STRENGTH FOR SUSTAINABLE CONSTRUCTION

ABSTRACT

This study aims to predict the compressive strength of mortars produced with GBFS and SMS. A total of 72 samples were prepared using six mixture ratios and four Na_2SiO_3 dosages and cured at 75 °C for 24 h. The dataset was analyzed using multivariate regression and machine learning models. Among regression approaches, the power function performed best (RMSE $\approx$ 4.9204 MPa, NSE $\approx$ 0.9284). However, the Gaussian Process (GP) model outperformed all other methodologies with the lowest prediction error and exceptional correlation (RMSE $\approx$ 1.4203 MPa, NSE $\approx$ 0.9920).

Keywords: Geopolymer mortar; compressive strength; machine learning; gaussian process; Monte Carlo cross-validation

INTRODUCTION

Steel has historically been the preferred material in many industrial sectors, owing to its superior mechanical properties, particularly its high strength and toughness. These characteristics render steel an indispensable material in construction, transportation, and a wide range of engineering applications. The iron and steel industry is critical to national economies, as it is a primary supplier of raw materials to key sectors such as manufacturing and infrastructure [1–3].

It is estimated that the production of each ton of steel generates approximately 400 kilograms of solid by-products, with the majority consisting of slag, which accounts for 70–80% of the total. Presently, these by-products are predominantly repurposed as secondary raw materials, with considerable potential for further utilization in various industries. Research has demonstrated the efficacy of utilizing steel slag in a variety of applications, including cement production, road construction, and civil infrastructure development [4–7].

The present study focuses on the potential reuse of by-products derived from steel production, particularly steel slags. The usability of these materials is heavily influenced by the cooling process, which affects their structural properties. The rapid cooling process, which typically involves substantial amounts of water, results in the formation of an amorphous, glass-like structure. The material produced through this process, with grains measuring approximately 4 mm in diameter, is referred to as granulated blast furnace slag (GBFS).

Despite GBFS exhibiting a lower rate of hydration than conventional Portland cement (OPC), numerous studies have shown that its integration into concrete mixtures results in substantial improvements in material performance. These include enhanced durability, improved corrosion resistance, reduced permeability, and enhanced workability [8–10].

Moreover, chemical activators have been demonstrated to augment the binding potential of pozzolanic materials, including slag and fly ash. The incorporation of these materials as sustainable alternatives to conventional cementitious binders is currently under investigation [11,12].

One of the most critical mechanical properties of conventional concrete, particularly those made with OPC, is compressive strength. This property constitutes the basis for structural design and load-bearing calculations. The preparation of concrete specimens is typically undertaken in accordance with standardized methodologies, such as those outlined in EN 12390-2, and the resultant specimens are then subjected to a curing process spanning 7-28 days, with the conditions of this process meticulously controlled. After the curing period, compressive strength tests are conducted to verify the material's compliance with the design requirements [13].

The timely prediction of compressive strength is crucial for ensuring the timely completion of projects and their structural safety. However, accurately determining the compressive strength at early ages remains challenging due to the time-dependent nature of cement hydration, particularly the formation of calcium-silicate-hydrate (C-S-H) gel. The process necessitates optimal moisture conditions and a suitable curing environment [14–16].

To overcome these challenges, several accelerated curing techniques have been developed, including autoclaving (steam curing), high-temperature curing, and hot-air curing. While these methodologies have proven efficacious in controlled laboratory environments, their practicality and cost-effectiveness for on-site implementation are often questionable. While 7-day compressive strength is frequently utilized as an early-age predictor of the 28-day strength, definitive structural validation remains contingent on the standard 28-day testing [17].

The limitations of conventional testing methods, including time constraints, financial costs, and labor-intensive procedures, have driven the escalating adoption of data-driven modeling approaches. These models, built on experimental data, have proven effective at predicting the mechanical properties of both traditional and alternative binders, such as geopolymers. The primary focus of these approaches is predicting parameters such as compressive, tensile, and flexural strengths [18,19].

Among the data-driven techniques, artificial intelligence (AI) has emerged as a powerful tool for predicting material performance with high accuracy. A variety of AI methodologies have been employed with considerable success, including the following:

The following essay will explore the application of Artificial Neural Networks (ANNs) in a variety of contexts [15].

- Fuzzy Logic (FL)
- Support Vector Machines (SVM)
- Genetic Algorithms (GA)
- Response Surface Methodology (RSM)
- Adaptive Neuro-Fuzzy Inference Systems (ANFIS)
- Genetic Programming (GP)
- Gene Expression Programming (GEP)

The efficacy of these AI-based methods in addressing complex, non-linear engineering problems has been well documented [20,21]. Artificial Neural Networks (ANNs) have gained prominence for their ability to learn and model nonlinear relationships. In addition to artificial

neural networks (ANNs), statistical methods such as multivariate regression have been used to predict compressive strength and other material properties. The versatility, adaptability, and robustness of AI-driven approaches render them highly reliable tools for modeling complex material behavior [22].

The objective of the present study is to ascertain the following:

The primary objective of this research is to develop accurate predictive models for the compressive strength of geopolymer mortars made with two industrial by-products: granulated blast furnace slag (GBFS) and steel mill slag (SMS). The experimental variables of slag content, activator dosage, and compressive strength were measured to develop and validate predictive models for these mortars. This study used GBFS and SMS as binders, mixed in 6 different ratios by substituting one for the other. Additionally, four different activator (Na_2SiO_3) ratios were tested, yielding 72 unique mortar samples. After measuring compressive strength, these samples were cured at 75°C for 24 hours. This study focuses on predicting compressive strength in geopolymeric mortars by examining the relationships between the percentage ratios of two supplementary cementitious materials (GBFS and SMS) and the alkali activator ratio, as independent variables. Compressive strength is considered the dependent variable. Linear, power, and exponential regression techniques, along with lightweight machine learning models such as Artificial Neural Networks (ANNs), were applied for predictive modeling. A review of the literature reveals the existence of strength-prediction models for geopolymeric mortars incorporating various admixtures. However, studies specifically investigating the combined effect of two different slags and developing dedicated models for compressive strength prediction remain limited. This research seeks to bridge this gap, offering a unique contribution to the field. Moreover, the early prediction of compressive strength eliminates the need to wait 7–28 days for conventional tests, providing significant economic and time-saving benefits.

MATERIALS AND METHODS

Materials

The blast furnace slag came from the Iskenderun Iron and Steel Plant, and the steel mill slag was from the Karabük Kardemir Iron and Steel Plant. Table 1 outlines their physical and chemical properties.

Table 1. Chemical and physical properties of BFS and SMS

Ingredients	BFS	SMS	Ingredients	BFS	SMS
SiO_2	38.89	13.53	BaO	0.45	-
CaO	28.94	52.83	P_2O_5	0.41	0.50
Al_2O_3	13.48	3.16	Na_2O	0.36	0.02
MgO	5.53	5.49	SrO	0.10	0.03
SO_3	1.51	0.99	V_2O_5	-	0.77
Fe_2O_3	1.36	12.74	Loss of Glow	6.50	7.24
MnO	1.16	1.73	Density (g/cm^3)	2.90	3.18
K_2O	0.78	0.16	Specific surface area	5980	6890
TiO_2	0.53	0.58	(g/cm^2)		

TEKKIM supplied the sodium silicate (Na_2SiO_3) used as the alkaline activator, and its properties are listed in Table 2.

Table 2. Activator properties

Parameters	Ratio
Purity	$\geq 95.0\%$
Na ₂ O	48 – 51
SiO ₂	44.4 – 47.4
Fe	≤ 0.1
Water Insoluble	≤ 0.5
pH	> 12.0
Melting temperature	1089 °C

Potable clean municipal water was used in the mortar mixtures [23], and the aggregate was ground river sand (0-3 mm).

Preparation of Geopolymer Mortars

Geopolymer mortar specimens were cast in prismatic molds with $40 \times 40 \times 160$ mm dimensions by the TS EN 196-7 standard [24]. The binder system comprised granulated blast furnace slag (GBFS) and steel mill slag (SMS), blended in six distinct proportions ranging from 100% GBFS–0% SMS to 0% GBFS–100% SMS, maintaining a constant total binder mass of 450 g. A fixed water-to-binder (w/b) ratio of 0.50 was employed throughout all mix designs to ensure consistency. Fine-crushed river sand was used as the inert aggregate. The precise proportions of the mixture and the detailed experimental design are outlined in Table 3. The concentration of the alkaline activator, sodium silicate (Na₂SiO₃), was varied relative to the binder mass at 3%, 6%, 9%, and 12%. Following the mixing stage, all specimens were subjected to thermal curing in a controlled oven environment at 75°C for 24 hours. Subsequent testing included a compressive strength evaluation conducted in accordance with TS EN 196-1 [24]. Statistical analysis was performed using SPSS software, with compressive strength as the dependent variable. The independent variables included the percentages of GBFS and SMS, and the activator dosage.

Three functions of classical regression analysis (power, exponential, and linear) and machine learning models (GP, SVM, and ANN) were employed to meet the research objectives. These approaches identified the model with the highest predictive accuracy for compressive strength and provided valuable insights into the factors influencing this critical mechanical property.

Table 3. Geopolymer mortar mixture design

No	SMS (%)	GBFS (%)	Na (%)	No	SMS (%)	GBFS (%)	Na (%)
1	100	0	3	13	40	60	3
2	100	0	6	14	40	60	6
3	100	0	9	15	40	60	9
4	100	0	12	16	40	60	12
5	80	20	3	17	20	80	3
6	80	20	6	18	20	80	6
7	80	20	9	19	20	80	9
8	80	20	12	20	20	80	12
9	60	40	3	21	0	100	3
10	60	40	6	22	0	100	6
11	60	40	9	23	0	100	9
12	60	40	12	24	0	100	12

Methodology of Modeling

This study establishes a comprehensive modeling framework by integrating classical regression techniques and machine learning algorithms to evaluate their predictive performance for estimating the mechanical properties of sustainable concrete mixtures incorporating industrial by-products. The modeling strategy is structured into three main categories: (i) classical models, including linear, power, and exponential regression, which provide interpretable baseline relationships through predefined mathematical functions; (ii) machine learning approaches, such as Gaussian Process (GP), Support Vector Machine (SVM), and Artificial Neural Networks (ANN), which offer flexible, data-driven modeling capabilities without strict assumptions about underlying patterns. This hierarchical comparison enables a systematic assessment of model accuracy, robustness, and generalization across varying levels of model complexity. The comparative analysis aims to identify the most suitable modeling approach for predicting key performance indicators in sustainable concrete applications, while highlighting the trade-offs between model interpretability, computational efficiency, and predictive accuracy.

Application of models

The study included four variables: one dependent variable (C_s , representing the actual compressive strength) and three independent variables (steel mill slag [SMS], blast furnace slag [BFS], and sodium metasilicate [NA]). Initially, the data collected from 72 experimental samples were normalized in Microsoft Excel to ensure consistency and comparability across the dataset [15].

Before their implementation in subsequent modeling analyses, the datasets were standardized within a range of 0.1 to 0.9. This normalization process effectively reduced the computational burden of outlier prediction and facilitated model optimization, thereby enhancing predictive performance and accuracy. The normalization was performed using the equation outlined in Equation [1], which ensures that the data inputs align within the specified range for model training.

$$\text{Normalised value} = \left[\frac{\text{Raw value} - \text{Minimum value}}{\text{Maximum value} - \text{Minimum value}} \right] \times (0.8) + 0.1 \quad (1)$$

The experimental data were partitioned into two subsets: 80% for training and 20% for testing, within a Monte Carlo cross-validation framework. This procedure was repeated 10 times to ensure statistical robustness and to minimize bias arising from data partitioning in the relatively small dataset. The regression and artificial neural network (ANN) models were constructed on the training set, and their accuracy was subsequently evaluated on the test set. The model's performance was evaluated using a range of quantitative metrics, including root mean square error (RMSE), mean absolute error (MAE), and Nash-Sutcliffe efficiency (NS). The assessment procedure is outlined below: [25,26]:

$$RMSE = \left[\frac{1}{n} \sum_{i=1}^n (O_i - P_i)^2 \right]^{1/2} \quad (2)$$

$$MAE = \frac{1}{n} \sum_{i=1}^n |O_i - P_i| \quad (3)$$

$$NS = 1 - \frac{\sum_{i=1}^n (O_i - P_i)^2}{\sum_{i=1}^n (O_i - \bar{O})^2} \quad (4)$$

Conventional regression analysis (CRA) is a widely used statistical estimation technique for modeling relationships between two or more variables using a predefined mathematical function. When the dataset comprises a single independent variable and a single dependent

variable, this methodological approach is known as univariate regression analysis. Conversely, the analysis is termed multivariate regression when multiple independent variables are considered simultaneously. The present study uses multivariate regression analysis to identify the optimal coefficients for three distinct regression models. The models under investigation include the linear function (LF), the power function (PF), and the exponential function (EF), with their respective mathematical formulations detailed in Equations 5–7 [18,21].

$$y_{Lf} = w_0 + w_1x_1 + w_2x_2 + w_3x_3 + \dots + w_n x_n \quad (5)$$

$$y_{pf} = w_0x_1^{w_1}x_2^{w_2}x_3^{w_3}x_4^{w_4}\dots x_n^{w_n} \quad (6)$$

$$y_{exp} = w_0 + \exp(w_1 + w_2x_1 + w_3x_2 + \dots + w_nx_n) \quad (7)$$

Drawing inspiration from the human brain's neural organization, artificial neural networks (ANNs) are computational models engineered to learn and represent the underlying relationships within datasets. These models can effectively map independent variables to dependent variables based on the patterns discerned during the training phase. Consequently, a well-trained ANN can generate accurate predictions from experimental or observational data. In contrast to traditional numerical analysis approaches, a suitably trained ANN can offer enhanced reliability and efficiency, while reducing computational requirements [15,27,28]. One of the primary advantages of ANNs is their ability to model complex systems with many independent variables, often with fewer constraints [29]. The first step in building an effective ANN model is to define its architectural structure. This involves determining the number of layers and the number of neurons per layer, both of which are crucial to model performance. These components are then integrated into the model by selecting suitable activation functions and values [15,18,30]. Furthermore, the performance of an ANN is heavily influenced by the quality and quantity of the training data. The model's generalization capability improves when the data is diverse and representative of the problem. The ANN method is widely applicable across various fields, including finance, healthcare, engineering, and social sciences, and is a valuable tool for solving complex problems [15,31]. To prevent overfitting, a minimal architecture with a single hidden layer and a limited number of neurons was selected, balancing model flexibility and generalization.

Gaussian Process (GP) is a non-parametric machine learning approach that models data through a probabilistic distribution rather than assuming a fixed functional form. Instead of fitting a predefined equation, GP defines a distribution over an infinite number of possible functions that could explain the observed data [32]. This is achieved using a kernel function, which computes the covariance between data points based on their similarity, forming a covariance matrix that guides both predictions and their associated uncertainty estimates. A key advantage of GP is its ability to provide not only point predictions but also confidence intervals, making it highly suitable for regression tasks with noisy or sparse data. Unlike classical regression models, GPs do not produce a single analytical formula; instead, they construct a flexible, data-driven probabilistic model that adapts to the underlying patterns in the data [32].

Support Vector Machine (SVM), particularly in its regression form known as ϵ -Support Vector Regression (ϵ -SVR), is based on the principle of structural risk minimization (Smola & Schölkopf, 2004). SVM maps input data into a higher-dimensional feature space using kernel functions (e.g., RBF or polynomial), enabling the modeling of nonlinear relationships through linear solutions in this transformed space. The method aims to fit a function that deviates from the target values by no more than a predefined threshold (ϵ), while minimizing model complexity to enhance generalization. Only data points outside this ϵ -tube contribute to the

error and influence the model, which helps prevent overfitting. SVM is particularly effective in small to medium-sized datasets and performs robustly under various data conditions. Unlike traditional regression techniques, SVM does not yield a fixed mathematical equation; instead, it builds a unique decision function based on support vectors and kernel-driven transformations learned from the data [33].

In this study, Monte Carlo cross-validation (MCCV) was employed to rigorously assess the predictive performance and stability of the proposed model. Unlike k-fold cross-validation, which uses deterministic data partitions, MCCV relies on repeated random subsampling: the dataset is split into training (80%) and testing (20%) subsets across 10 independent iterations. This approach provides a robust evaluation framework by exposing the model to diverse data configurations, thereby capturing the variability in performance that may arise from different sampling realizations. The use of Monte Carlo cross-validation is particularly justified in this context to ensure that the model's performance is not overly optimistic or biased due to a single, potentially favorable train-test split, especially in datasets with inherent heterogeneity or limited size. In each iteration, the model was trained on the training subset and evaluated on the test subset using key regression metrics: Root Mean Square Error (RMSE), Mean Absolute Error (MAE), and Nash-Sutcliffe Efficiency (NSE). The results across all iterations were aggregated and reported in terms of mean (to represent average performance), standard deviation (to quantify variability and model robustness), minimum and maximum values (to illustrate the range of possible outcomes), and the best observed result (to identify the most favorable performance scenario). This comprehensive statistical summary not only highlights the central tendency of model accuracy but also reveals its sensitivity to data fluctuations, offering a transparent and reliable assessment of its generalization capability in real-world applications.

Furthermore, Monte Carlo Cross-Validation (MCCV) significantly mitigates the risk of overfitting by exposing models to multiple independent train-test splits. In particular, the Gaussian Process model inherently incorporates regularization through its kernel-based covariance structure, thereby constraining model complexity and preventing overfitting even with small datasets. The low standard deviation observed across iterations further confirms the stability and generalization capability of the proposed modeling framework.

Model hyperparameters and implementation details

To ensure the reproducibility of the results and address the specific configurations of the machine learning models, the following hyperparameter settings and optimization methods were employed:

- **Gaussian Process Regression (GPR):** The GPR model was implemented using the Squared Exponential (Radial Basis Function - RBF) kernel. The hyperparameters, including the signal standard deviation and the characteristic length scale, were optimized using the Exact GPR method to ensure the highest predictive accuracy for the geopolymer mortar dataset. The hyperparameters were optimized by maximizing the log-marginal likelihood, including the characteristic length scale and noise variance parameters, thereby ensuring the model's reproducibility and numerical stability.
- **Support Vector Machines (SVM):** The SVM model utilized a Gaussian kernel (RBF) to handle the nonlinear relationships between the geopolymer components and compressive strength. The model was trained using the Sequential Minimal Optimization (SMO) solver, and the box constraint (insensitive tube) was automatically tuned to minimize the epsilon-loss function during training.

- Artificial Neural Networks (ANN): A feed-forward backpropagation network architecture was selected, consisting of a single hidden layer with 5 neurons as optimized during preliminary trials. The Levenberg-Marquardt (LM) algorithm was used for training due to its efficiency in small datasets, and the Log-Sigmoid transfer function was applied in the hidden layer to capture nonlinearities.

RESULTS AND DISCUSSION

CRA test results

In this study, 3 regression functions were applied. The effect coefficients of these functions are given in Table 4. The model performance statistics are given in Table 5. The model with the best results is in bold. The comparison between actual values and predicted data is shown in Figure 3. Looking at the performance statistics, the best results are obtained with the power function. Regarding the RMSE, MAE, and NSE metrics, the Power Function (PF) demonstrated the most robust performance among the conventional regression methods when evaluated across both the training and test phases within the Monte Carlo cross-validation framework.

The predictive stability and accuracy of the Power Function, identified as the most robust approach among the classical regression methods, are evaluated through 10 independent iterations. The alignment between the experimental measurements and the predicted values during the training phase is illustrated in Figure 1. At the same time, the model's generalization capability on the test dataset is shown in Figure 2. Furthermore, the overall regression accuracy and correlation across all experimental data points are visually summarized in the scatter plots shown in Figure 3.

Table 4. Coefficients for functions used in the CRA method

Model	w0	w1	w2	w3	w4
Linear Function	-9.40809586	60.75646216	0	30.68525639	
Power Function	93.90347679	0.815688972	0.050781194	0.36487679	
Exponential Function	-33.0490631	63.67480222	-59.26454503	-60.12329955	0.4438

Table 5. Performance statistics of the CRA method

CRA		RMSE (MPa)		MAE (MPa)		NSE	
		Train	Test	Train	Test	Train	Test
Linear	Ave.	5.1121	5.6094	3.9162	4.4871	0.9298	0.9093
	Std.	0.1939	0.6294	0.1833	0.5109	0.0070	0.0345
	Best	4.7737	4.8157	3.6211	3.6984	0.9409	0.9437
Power	Ave.	4.8744	4.9204	3.8097	3.8849	0.9361	0.9284
	Std.	0.2412	0.8692	0.2283	0.7049	0.0080	0.0337
	Best	4.5454	3.9592	3.3999	3.1690	0.9467	0.9635
Exp.	Ave.	5.4979	6.1383	4.0793	4.7982	0.9188	0.8926
	Std.	0.2540	0.7566	0.2678	0.4879	0.0092	0.0347
	Best	5.2318	5.2876	3.8354	4.2029	0.9306	0.9302

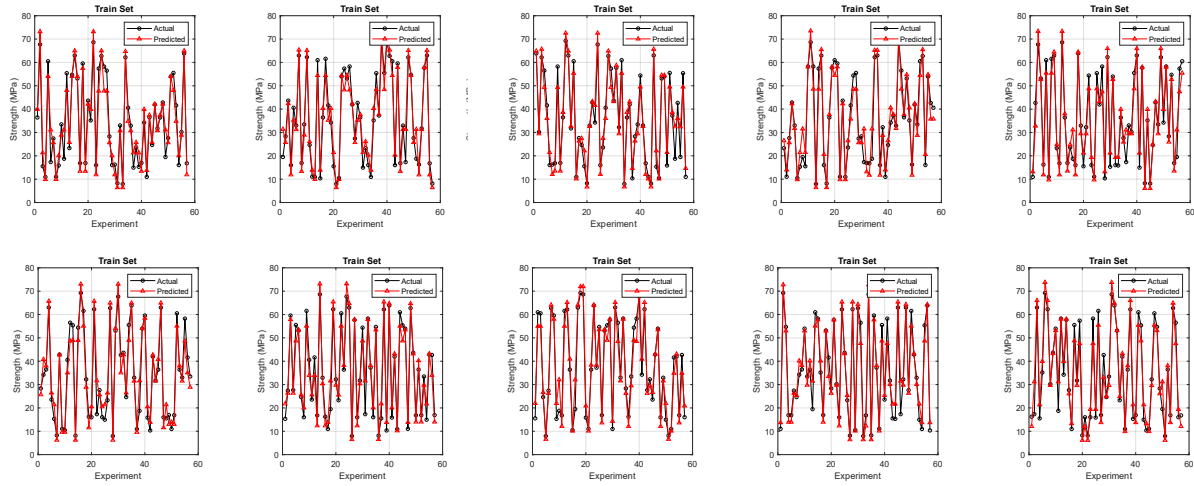


Fig. 1. Iterative performance analysis of the Power Function regression: Comparison between experimental results and predicted compressive strength for the training dataset

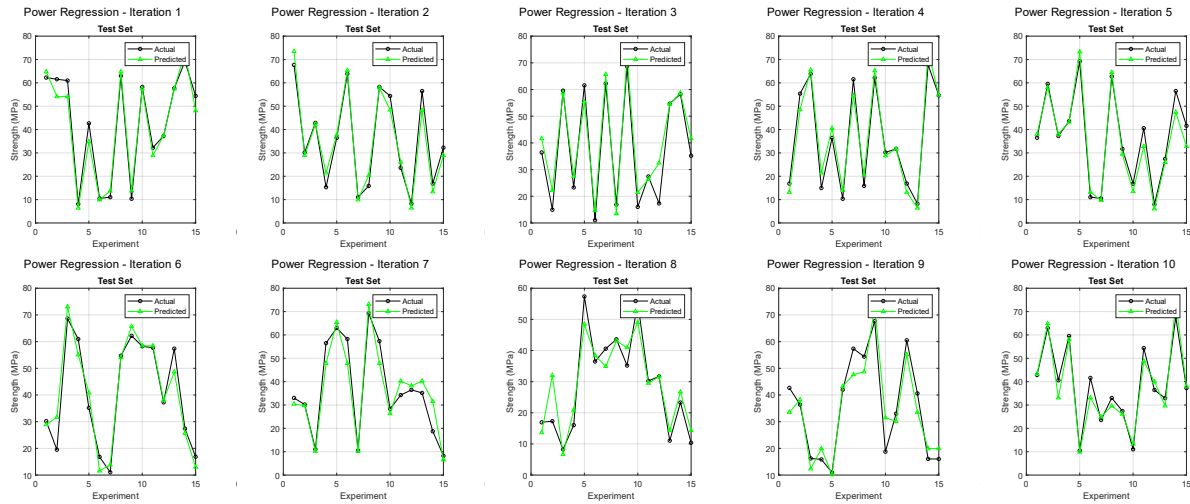


Fig. 2. Prediction performance of the Power Function model on the testing dataset: Evaluation of prediction stability across 10 independent iterations

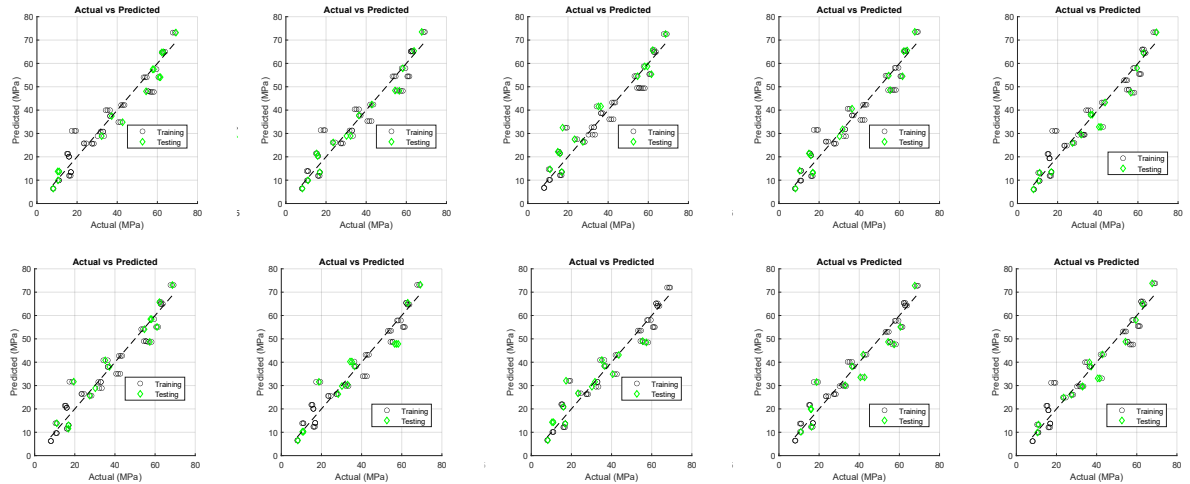


Fig. 3. Regression accuracy of the Power Function approach: Actual vs. predicted scatter plots for all experimental data points

ANN, SVM, and GP Test results

The performance statistics of the ANN, SVM, and GP models are given in Table 6. The model with the best results is in bold. The comparison between actual values and predicted data is shown in Figure 4. Examining the performance statistics of the ANN, SVM, and GP models reveals that the GP model yields the best results. For the RMSE, MAE, and NSE indicators, the Gaussian Process (GP) model achieved the superior overall results. The model exhibited exceptional predictive accuracy and stability when the training and test datasets were combined across all 10 independent iterations.

The Gaussian Process (GP) model demonstrated exceptional predictive performance, outperforming all other artificial intelligence-based methodologies. The iterative performance analysis of the training dataset is detailed in Figure 4, demonstrating high-fidelity tracking of the experimental results. The model's superior stability on unseen testing data across all 10 iterations is evidenced in Figure 5. The high degree of alignment and minimal variance between actual and predicted regression accuracy plots in Figure 6 further validate compressive strength values.

Table 6. Performance statistics of the ANN methods

ML		RMSE (MPa)		MAE (MPa)		NSE	
		Train	Test	Train	Test	Train	Test
SVM	Ave.	5.4767	5.9064	4.0450	4.5123	0.9195	0.9009
	Std.	0.1955	0.6987	0.1655	0.5224	0.0076	0.0331
	Best	5.1682	4.4449	3.7978	3.3695	0.9327	0.9283
GP	Ave.	0.5432	1.4203	0.4158	1.0148	0.9992	0.9920
	Std.	0.0291	1.0025	0.0208	0.5379	0.0001	0.0138
	Best	0.5064	0.9372	0.3846	0.7203	0.9994	0.9979
ANN	Ave.	3.3037	4.0679	2.1562	2.7635	0.9663	0.9446
	Std.	1.3864	1.9388	0.8441	1.0934	0.0275	0.0550
	Best	1.7448	1.6721	1.2916	1.1715	0.9921	0.9916

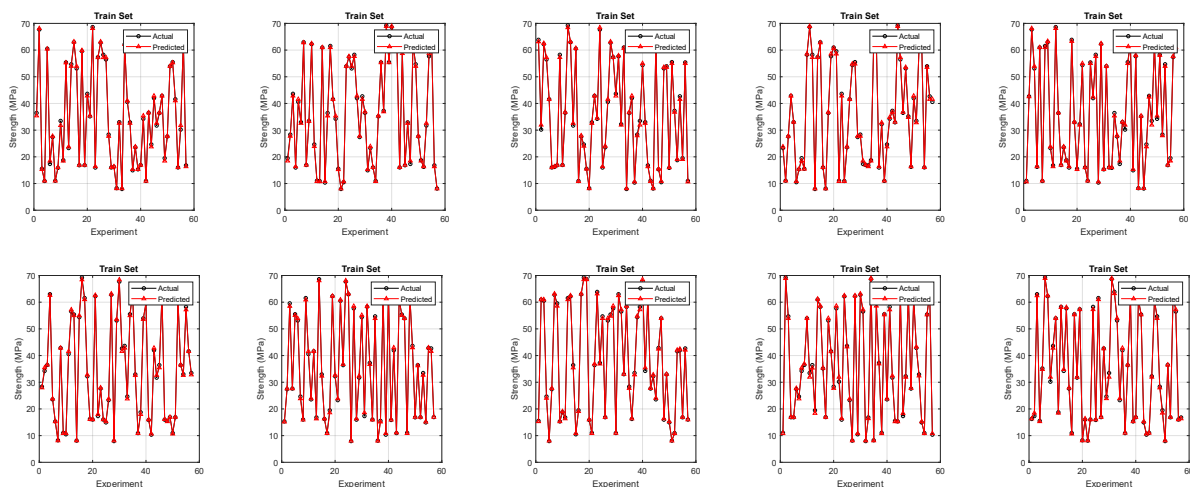


Fig. 4. Iterative performance analysis of the Gaussian Process (GP) regression: Comparison between experimental results and predicted compressive strength for the training dataset

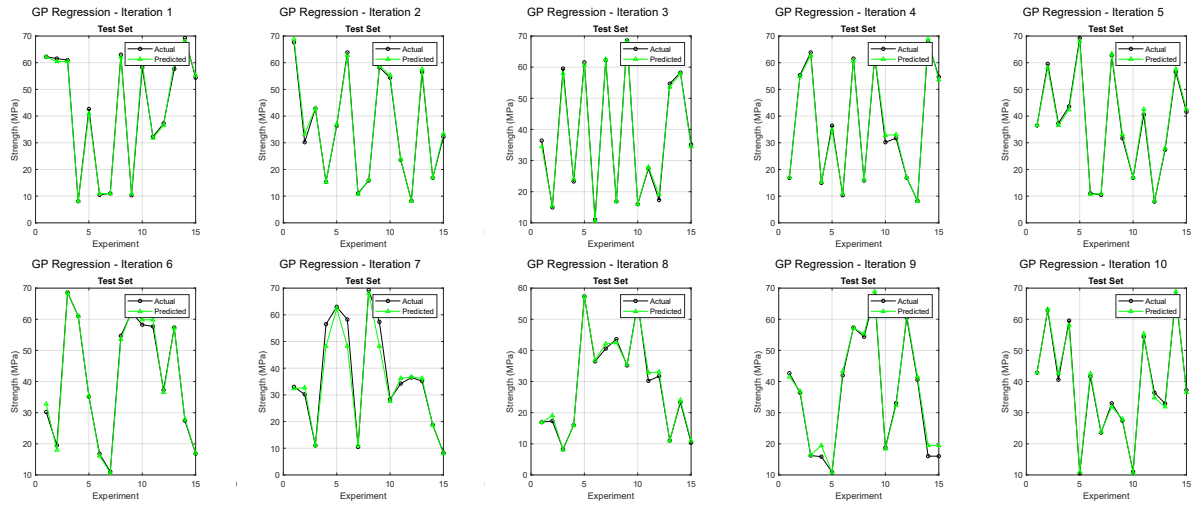


Fig. 5. Prediction performance of the Gaussian Process (GP) model on the testing dataset: Evaluation of prediction stability across 10 independent iterations

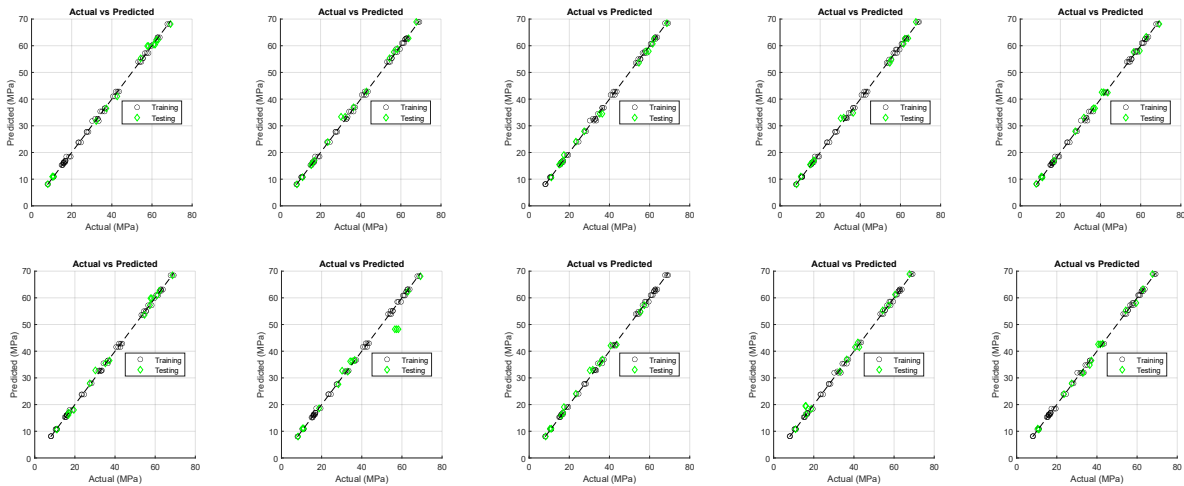


Fig. 6. Regression accuracy of the Gaussian Process (GP) approach: Actual vs. predicted scatter plots for all experimental data points

To provide a comprehensive comparative evaluation of the developed models, a Taylor diagram was constructed as shown in Figure 7. This diagram facilitates a multi-criteria statistical assessment by simultaneously visualizing the Pearson correlation coefficient, the normalized standard deviation, and the root-mean-square (RMS) error for each model relative to the experimental reference point. The Taylor diagram clearly demonstrates the superiority of the Gaussian Process (GP) model, which is positioned closest to the reference point, indicating the highest correlation and the lowest centered RMS error. While the Power function and ANN models show competitive performance, the GP model's proximity to the actual experimental variance highlights its exceptional capacity to capture the complex, non-linear relationships within the SMS-GBFS geopolymer system, even with a limited sample size.

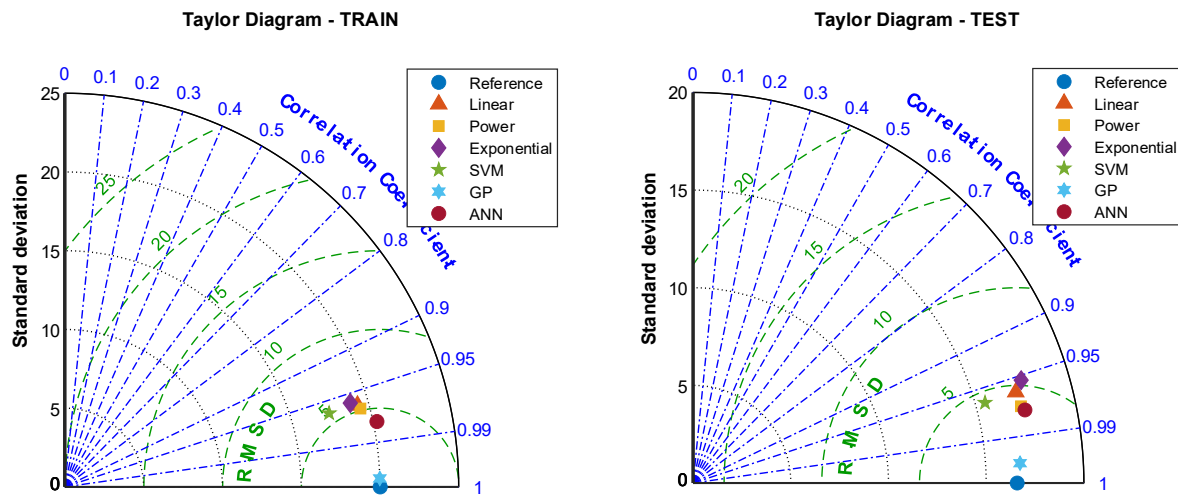


Fig. 7. Taylor diagram illustrating a multi-criteria statistical comparison of the developed models based on Pearson correlation, normalized standard deviation, and root-mean-square (RMS) error

To provide a definitive quantitative comparison, the overall statistical performance of all predictive models is consolidated in Figure 8. This summary visualization highlights the error distribution (RMSE and MAE) and predictive efficiency (NSE) for each methodology across the Monte Carlo cross-validation cycles. It is evident that while classical regression models like the Power function provide a reasonable baseline, the Gaussian Process (GP) model consistently maintains the lowest error margins and the highest correlation values in both training and testing phases. The narrow gap between the training and testing metrics in Figure 8 further validates that the GP and ANN models, as implemented in this study, are highly resilient to overfitting, ensuring reliable strength predictions for sustainable geopolymers design.

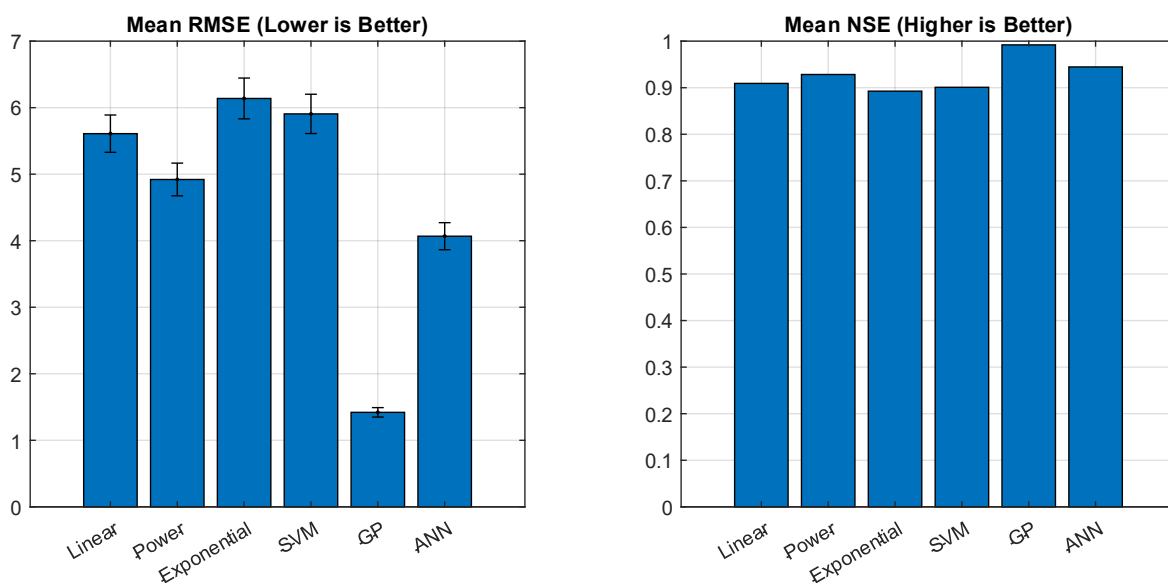


Fig. 8. Comprehensive performance summary of all developed models: Comparative analysis of RMSE, MAE, and NSE metrics for training and testing datasets across 10 iterations

CONCLUSIONS

The present study proposes a comprehensive modeling approach to predict the compressive strength of geopolymer mortars produced using industrial by-products, such as granulated blast furnace slag (GBFS) and steel mill slag (SMS). The ability of the aforementioned models to predict the mechanical properties of geopolymer mortars was evaluated through analyses employing traditional regression analyses (linear, exponential, power) and machine learning algorithms (ANN, SVM, GP). The findings revealed the comparative performance of different modeling approaches and made significant contributions to the field's knowledge base.

The primary outcomes of this study can be summarized as follows:

- In the context of conventional regression models, the power function exhibited the best performance for predicting the compressive strength of geopolymer mortars. The root mean square error (RMSE), mean absolute error (MAE), and Nash–Sutcliffe efficiency (NSE) values confirmed that the power function provided reliable predictions for both the training and test datasets. This result highlights that even comparatively simple mathematical formulations can yield satisfactory strength predictions within suitably defined domains [15,34].
- Regarding machine learning models, Gaussian Processes (GP) outperformed all other methodologies, including Artificial Neural Networks (ANN) and Support Vector Machines (SVM), in predicting compressive strength. The GP model achieved the lowest error indices and the highest goodness-of-fit coefficients among all tested models. Its probabilistic nature and its ability to provide uncertainty estimates offered a clear advantage for modeling the complex, highly nonlinear behavior of geopolymer mortars [15,35].
- Overall, the study has shown that a wide spectrum of modeling techniques can be effectively employed to predict the compressive strength of geopolymer mortars. While traditional regression methods with power-type functional forms offer reasonable accuracy, advanced machine learning approaches such as GP achieve considerably higher predictive performance and robustness. These findings emphasize the importance of data-driven modeling strategies for the design, development, and optimization of sustainable geopolymer-based materials in the construction industry [36].

Future work should focus on improving the generalisability of the proposed models by validating them on larger, more diverse datasets that encompass different mix proportions and curing conditions. In addition, more detailed investigations into the influence of various industrial by-products and chemical activators on model performance are recommended. The broader adoption of geopolymer mortars supported by such predictive tools is expected to contribute significantly to environmental sustainability by reducing CO₂ emissions and enabling more efficient material design.

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