EPH–International Journal of Science & Engineering
Published by: E-Pub Solutions Private Limited
ISSN (Online): **2454-2016**
Volume 12 Issue 03 August 2026
DOI:10.67772/7gvcmn02

DATA-DRIVEN PREDICTION OF MECHANICAL STRENGTH AND ELECTRICAL RESISTIVITY IN GRAPHITE-MODIFIED CEMENTITIOUS COMPOSITES

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Article History:
Article Type: Research
Received Date: **04/07/2026**
Revised Date: **06/08/2026**
Accepted Date: **15/08/2026**
Published Date:**25/08/2026**

Keywords: Graphite-modified cementitious composites; Unconfined compressive strength; Electrical resistivity; Machine learning; Predictive modeling

ABSTRACT

The present study proposed a data-driven machine learning approach for the prediction of mechanical strength and electrical resistivity of graphite-modified cementitious composites. The experimental data analyzed consisted of two independent sets: 373 observations of unconfined compressive strength (UCS) and 416 observations of electrical resistivity (ER), comprising graphitic-material properties, proportions of the mixtures, processing conditions and curing parameters. Six regression models – Linear Regression, Decision Tree, Random Forest, Gradient Boosting/ XGBoost, Support Vector Regression and K-Nearest Neighbors – were tested with cross-validation and an 80/20 train-test split. The performance of the models was evaluated based on R2, MAE, MSE, and RMSE. Random Forest gave the best fit to the model for the UCS prediction with an R^2 of 0.888, MAE of 3.75, MSE of 25.10 and RMSE of 5.01, while the best model for the ER prediction was Decision Tree, with an R^2 value of 0.991, MAE of 40.20, MSE of 1623.00, and RMSE of 67.58. The curing age, water-to-cement ratio, graphitic thickness, and ultrasonication strongly affected the UCS value, while the graphitic content, water-to-cement ratio, surface area, use of superplasticizer, and conditions related to the measurement had a more pronounced effect on the ER value. In general, it is shown that nonlinear machine-learning models are capable of capturing complex material-property relationships and are useful for optimizing the multifunctional and self-sensing cementitious composites.

Introduction

Cementitious materials are one of the most widely used construction materials around the world due to their ready availability, structural versatility, durability and relatively inexpensive production. However, the performance of conventional cement-based materials is limited for emerging multifunctional and smart infrastructure applications due to their brittle behavior, susceptibility to cracking, and inherently poor electrical conductivity. Therefore, a great deal of effort has been made to develop cementitious composites with carbon-based nanomaterials for the improvement of mechanical, durability, and functional properties (Shamsaei et al., 2018; Xu et al., 2018). Graphitic materials are especially promising, since their unique physical and electrical properties can alter the hydration, microstructure, crack propagation and conductive pathways of cement. For instance, graphene oxide (GO) affects hydration and microstructural development in ordinary Portland cement (OPC) (Chintalapudi & Pannem, 2020). These findings suggest significant potential for developing cementitious materials with both structural and desirable electrical properties.

The cementitious material can be modified by nanoscale reinforcement and pore refinement, nucleation effects, and formation of electrically conductive networks with the addition of graphite, graphene nanoplatelets, GO and related carbonaceous materials. Experimental studies have shown that after a proper amount of GO addition, the mechanical properties and microstructural characteristics are enhanced (Lee et al., 2020; Peng et al., 2019). Nano-graphite has also been reported to be useful in manufacturing of high-performance cementitious nanocomposites (Chougan et al., 2020). However, the dosage, dimensions, surface characteristics and dispersion quality of graphitic material have a significant effect on performance. An agglomeration leads to a decrease in the reinforcing effect, while the right dispersion causes better interaction with the cement matrix (Lu et al., 2019; Sabziparvar et al., 2019). So, surfactants and ultrasonication have been explored as means to enhance the dispersion of nanomaterials (Chuah et al., 2018; Gao et al., 2019). Further, hybrid graphene oxide and carbon nanotube systems clearly show that the proportions of reinforcement have a significant impact on the performance of composite systems (Du et al., 2020). It is important to optimize these additions as they impact both electrical resistivity and mechanical properties simultaneously when adding graphene to a composite (X. Li et al., 2018). The rheological behaviour and workability also have to be taken into consideration as adding graphitic additives may affect both the fresh state properties and the performance of the material afterwards (Alharbi et al., 2020; Suo et al., 2020).

Optimization is difficult with a purely empirical approach, due to the many interactions between characteristics of the graphitic materials, mixture proportions, processing conditions, curing parameters, and properties of the composite. Alternatively, data-driven statistical and machine-learning methods can be used to learn nonlinear relationships between the input parameters and material responses. These kinds of models potentially lower the number of experiments, use of materials and optimization time required for extensive laboratory testing to estimate mechanical strength and electrical resistivity. This method is important because the performance of cementitious materials containing graphene is highly sensitive to dispersion and processing conditions, and not just graphitic content (Chuah et al., 2018; Sabziparvar et al., 2019). Furthermore, the reported influences of the size of the aggregation, ultrasonication and hybrid reinforcement, have highlighted the multi-variable nature of these material systems (Gao et al., 2019; Lu et al., 2019).

Although many experimental studies have been conducted with graphene- and graphite-cementitious materials, the majority of the research focuses on one individual mechanical, microstructural, rheological, or electrical property. Research to create models of mechanical strength and electrical resistivity based on such data is still relatively scarce. The literature also shows significant sensitivity to the type of material, dosage, dispersion, and processing conditions (X. Li et al., 2018; Shamsaei et al., 2018). As a result, an integrated predictive investigation is needed to identify the major material and processing variables that affect the structural and electrical performance.

In this regard, the goal of this study is the building up of data-driven models for the prediction of the unconfined compressive strength (UCS) and electrical resistivity (ER) of the graphite-modified cementitious composites. It also aims to determine the most significant graphitic material, mixture, curing and processing parameters, and to compare the alternative predictive models based on the well-known regression performance metrics. The end goal of the study is to create a sound predictive model that facilitates the development of efficient material optimization and multifunctional cementitious composites.

2. Methodology
2.1 Research Design
The approach adopted in this study was quantitative data analysis and predictive design to predict mechanical and electrical properties of graphite-modified cementitious composites. Two regression tasks were designed; the first one predicting unconfined compressive strength (UCS) and the second one predicting electrical resistivity (ER). It was necessary to do separate modelling, as UCS and ER were both given in different datasets, but were not accompanied by a common specimen identifier.
2.2 Dataset Description
Two CSV files were analysed. There were 373 observations and 13 variables in the dataset and 416 observations and 14 variables in the ER.csv dataset (Dong, 2022). Both datasets contained experimental data for cementitious composites incorporating graphitic materials including graphene nanoplatelets (GNP), graphene oxide (GO) and reduced graphene oxide (rGO). These variables included material properties, mixture proportions, processing conditions and curing parameters.
2.3 Study Variables
Mechanical-property model: Dependent variable was UCS. Electrical-property model: Dependent variable was ER. The graphitic material type, the content of graphitic material, the dimension of the graphitic material, the thickness of the material, the surface area, the sand-to-cement ratio, the water-to-cement ratio, the use of superplasticizer, ultrasonication, curing environment, and curing age were used as predictor variables. The ER dataset also included an experimental measurement condition variable (AD).
2.4 Data Preprocessing
Before developing the models, both databases were checked for missing values, duplicate data, inconsistent data, and data types. There are no duplicate records were found. The missing data were primarily in the graphitic dimensions, thickness, surface area, and ultrasonication variables with the highest being the surface area of the graphitic dimension. Data points were dealt with appropriately with missing values replaced by training data imputations, and variables with significant missingness were carefully evaluated prior to inclusion. Categorical variables were one-hot encoded and numerical variables were scaled to the standard normal distribution for algorithms sensitive to the scale of the features.
2.5 Exploratory Data Analysis
Both UCS and ER were analysed separately using descriptive statistics and graphical analysis. Continuous variables were analysed in terms of mean, standard deviation, minimum and maximum values and categorical variables were analysed in terms of frequencies. Plots of the distribution were used to check the UCS and ER, and correlation analysis was used to check the relationships between the numerical predictors and target variables. Focus was placed on the following: graphitic content, water-to-cement ratio, curing age, dimensions and surface area.
2.6 Machine-Learning Models
The following six regression algorithms were tested: Linear Regression, Decision Tree Regression, Random Forest Regression, Gradient Boosting/XGBoost Regression, Support Vector Regression, and K-Nearest Neighbors Regression. The models chosen for comparison are conventional linear predictions and various tree-based, ensemble, kernel and distance-based models that can model nonlinear relationships.
2.7 Model Training and Validation
The dataset was separated into 80% training and 20% testing data for each target variable. The training subset was used for model development and hyperparameter tuning, and the testing subset was reserved to evaluate the models independently. To ensure the stability of the model and minimize reliance on a single data partition, cross-validation was used during training.
2.8 Model Performance Evaluation

The coefficient of determination (R^2), mean absolute error (MAE), mean squared error (MSE), and root mean squared error (RMSE) were used to evaluate model performance. The higher the R^2 values and the lower the values of MAE, MSE, and RMSE, the better the predictive performance. The metrics were computed independently for the UCS and ER models to explore the best algorithm for each prediction task.

2.9 Model Interpretation

The top-performing models were then analyzed with feature-importance analysis and SHapley Additive exPlanations (SHAP), if applicable. This analysis was employed to determine the most significant material, mixture, processing and curing variables to predict UCS and electrical resistivity. Special attention was given to the water-to-cement ratio, the environment for curing, the curing age, ultrasonic treatment, and graphitic material type and content, as well as the graphitic dimensions.

3. Results

3.1 Dataset and Material Characteristics

A total of 373 tests were performed for unconfined compressive strength (UCS) and 416 for electrical resistivity (ER). The UCS values ranged from 14.22 to 95.19, with a mean of 49.29 ± 17.30, whereas ER showed substantially greater dispersion, ranging from 0.15 to 2474.53, with a mean of 750.32 ± 723.94. The datasets comprised GNP-, GO-, and rGO-modified cementitious composites with variation in water-to-cement ratio, curing age, ultrasonication, graphitic dimensions, and other mixture and processing characteristics. There was significantly larger relative variability in ER than in UCS as shown in Table 1.

Table 1. Descriptive Characteristics of the UCS and ER Datasets

Dataset	Observations	Mean	SD	Minimum	Median	Maximum
UCS	373	49.29	17.30	14.22	49.00	95.19
ER	416	750.32	723.94	0.15	599.02	2474.53

3.2 Mechanical Strength Characteristics

There was a moderate variation in the distribution of UCS among the graphitic-material categories. The mean UCS for GNP, GO, and rGO was about 49.13, 48.51, and 52.76, respectively, with the mechanical strength of observations containing rGO being slightly higher. But the GO and GNP groups showed larger variation and rGO showed smaller variation. These differences are shown in Figure 1, and it is apparent that there was still significant within-group variation, indicating that, as well as the type of graphitic material, the mechanical performance of the materials was dependent on mixture proportions, curing conditions and material characteristics.

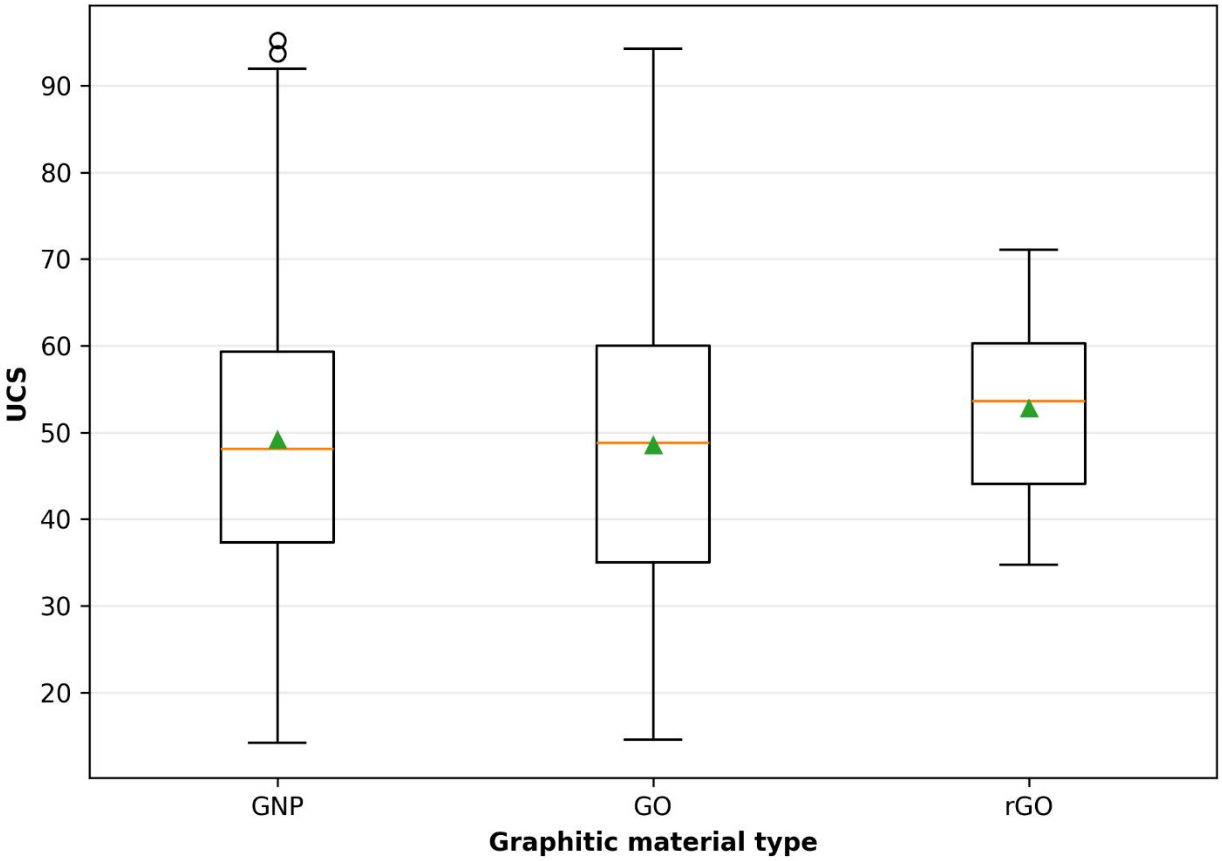

Figure 1. Distribution of Unconfined Compressive Strength According to Graphitic-Material Type

3.3 Electrical Resistivity Characteristics

Electrical resistivity differences were significant depending on the type of graphitic material. The mean ER of GNP-modified composites was the lowest (465.87) compared to the significantly higher mean values of 1099.14 and 1277.56 of GO and rGO composites, respectively. Median ER had a similar overall trend where GNP was 115.50 and GO and rGO were 1130.00 and 1578.38 respectively. Table 2 shows that a significant difference in electrical behavior was only related to material type, but the standard deviations were high and indicated that other effects were caused by dosage and mixture conditions.

Table 2. Electrical Resistivity According to Graphitic Material Type

Graphitic material	N	Mean ER	Median ER	SD	Minimum	Maximum
GNP	239	465.87	115.50	630.05	0.15	2136.63
GO	142	1099.14	1130.00	671.03	5.60	2474.53
rGO	35	1277.56	1578.38	622.65	118.48	1998.53

3.4 Relationships Among Material Variables

The mechanical strength and electrical resistivity showed different patterns of predictors in the correlation analysis. The curing age had the highest positive correlation ($r = 0.465$) with UCS, and the water-to-cement ratio had a moderate negative correlation ($r = -0.348$) with UCS. There was also a negative correlation between UCS and the S/C ratio ($r = -0.235$). On the contrary, ER was correlated with ultrasonication ($r = 0.492$) and graphitic content ($r = -0.454$) and graphitic dimension ($r = -0.431$) and water-to-cement ratio ($r = -0.344$). The two predictive outcomes have contrasting correlation structures, as shown in Figure 2.

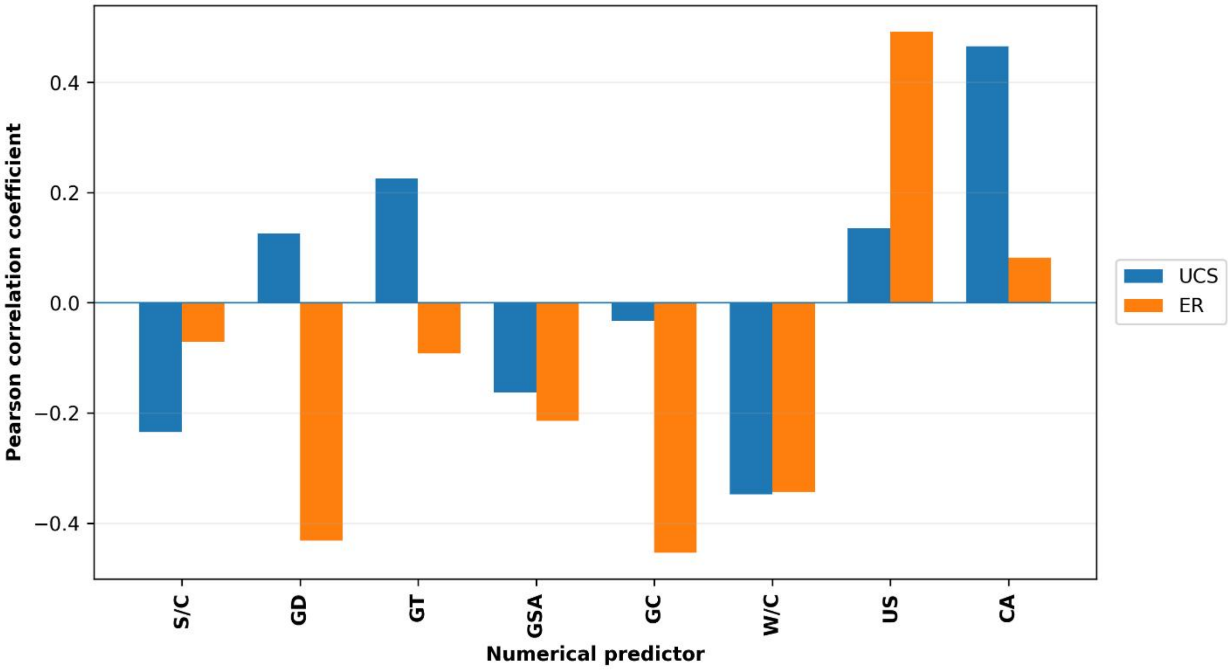

Figure 2. Correlations of Numerical Material Variables with UCS and Electrical Resistivity

3.5 Machine-Learning Performance for Mechanical Strength

All nonlinear machine-learning models outperformed Linear Regression for UCS prediction. Random Forest model was the best model with the highest test performance with R 2 of 0.888, MAE of 3.75, MSE of 25.10 and RMSE of 5.01. Gradient Boosting had a slightly higher cross-validation R 2 and lower test R 2 of 0.871, whereas Linear Regression had the lowest performance with the R 2 of 0.487. These results show that the dependence of mechanical strength on the parameters of mixtures was mostly nonlinear.

Table 3. Predictive Performance of Machine-Learning Models for UCS

Model	CV R^2	Test R^2	MAE	MSE	RMSE
Random Forest	0.865	0.888	3.75	25.10	5.01
Gradient Boosting	0.880	0.871	3.92	28.87	5.37
Decision Tree	0.832	0.808	4.59	43.01	6.56
SVR	0.774	0.801	5.17	44.57	6.68
KNN	0.856	0.776	4.78	50.19	7.08
Linear Regression	0.494	0.487	8.68	115.06	10.73

3.6 Machine-Learning Performance for Electrical Resistivity

Tree-based algorithms predicted the electrical resistivity with the highest accuracy. The Decision Tree model had the highest test R2 (0.991), MAE (40.20) and RMSE (67.58). Random Forest and Gradient Boosting were also impressive, with test R^2 values of 0.989 and 0.986, respectively. The Decision Tree model with the lowest error (Figure 3) exhibits strong agreement between observed and predicted ER with the majority of predictions being close to the identity line.

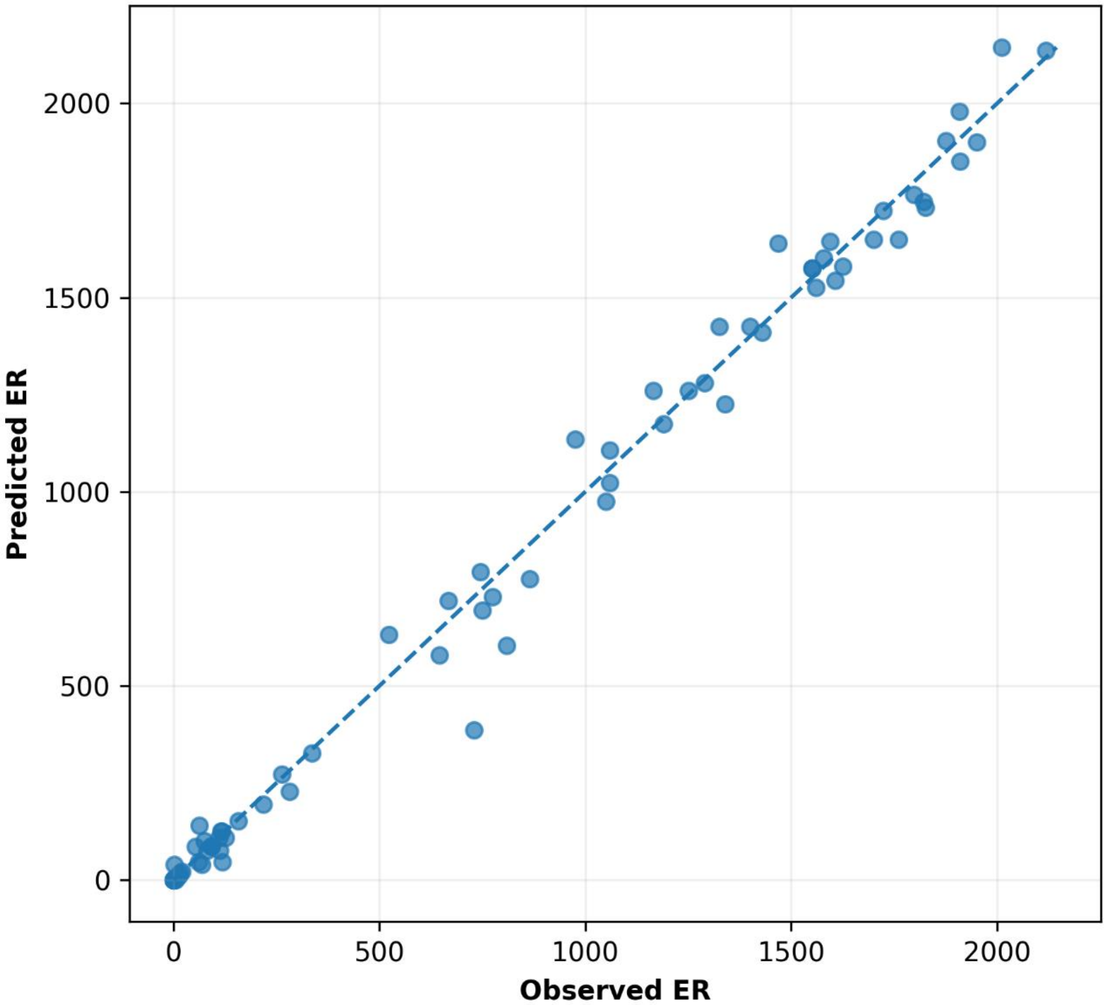

Figure 3. Observed Versus Predicted Electrical Resistivity for the Best-Performing Model

3.7 Feature Importance and Model Interpretation

The feature importance that was based on permutation showed different controlling variables for the two outcomes. In the case of UCS, the most significant predictor was curing age (0.607), then water-to-cement ratio (0.515), graphitic-material thickness (0.491), and ultrasonication (0.195). In the case of ER, the dominant graphitic content (0.951) was followed by water-to-cement ratio (0.678), AD (0.589) and graphitic surface area (0.239) and the use of superplasticizer (0.218). Table 4 thus suggests that the mechanical strength was mainly determined by curing and dimensional properties, and electrical resistivity was significantly determined by graphite dosage and mixture parameters.

Table 4. Permutation Feature Importance for the Best UCS and ER Models

Predictor	UCS importance	ER importance
Curing age (CA)	0.607	0.115
Water/cement ratio (W/C)	0.515	0.678
Graphitic thickness (GT)	0.491	0.061
Ultrasonication (US)	0.195	0.000
Graphitic content (GC)	0.046	0.951

Graphitic dimension (GD)	0.058	0.045
Graphitic surface area (GSA)	0.008	0.239
Superplasticizer (SP)	0.000	0.218
AD	—	0.589

3.8 Overall Predictive Findings

The data-driven framework provided satisfactory results overall with both mechanical and electrical resistivity being predicted with good accuracy, with ER having a much higher predictive accuracy. The best model for predicting UCS was the Random Forest model ($R^2 = 0.888$), while the best model for predicting ER was the Decision Tree model ($R^2 = 0.991$). The two material responses were also found to have different predictor structures using the feature-importance analysis. For UCS, the effects of curing age, W/C ratio, graphitic thickness, and ultrasonication were of particular importance, whereas graphitic content, W/C ratio, AD, surface area, and superplasticizer played the main role in the prediction of ER. These differences are illustrated in a comparative way in Figure 4 and this means it is important to model both outcomes separately and not presume the same governing mechanisms.

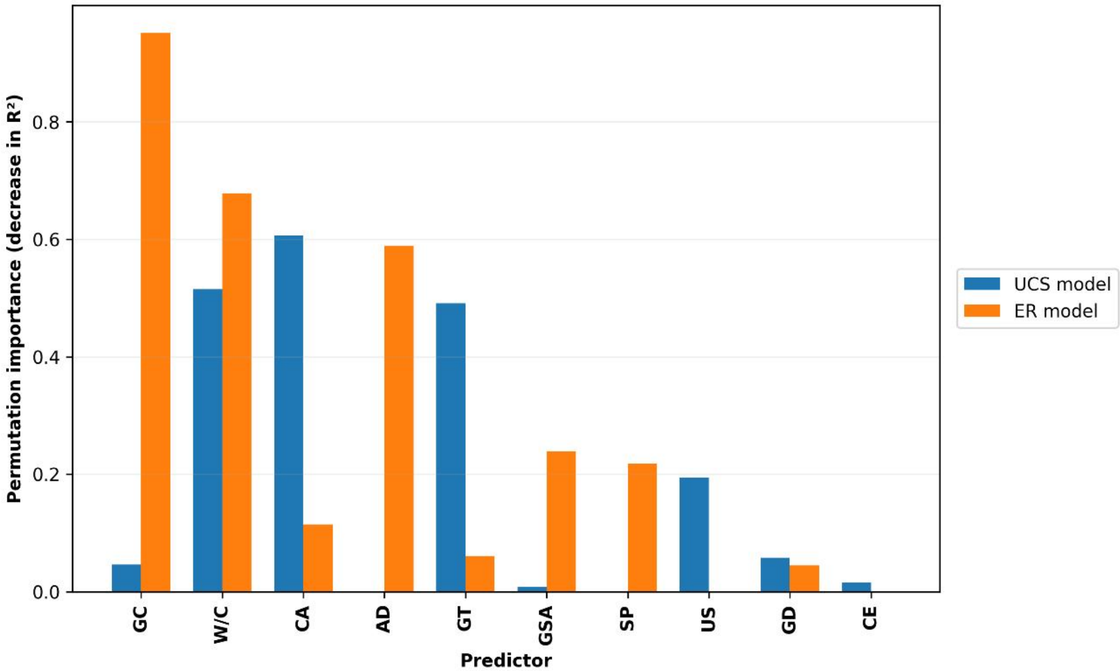

Figure 4. Comparative Permutation Importance of Predictors for UCS and Electrical Resistivity

4. Discussion

The results indicate that both mechanical strength and electrical resistivity of graphite-modified cementitious composites can be forecasted using data-driven approaches successfully. Random Forest model gave the best forecast for UCS (R2 = 0.888) and Decision Tree Regression for ER (R2 = 0.991). These findings support the idea that the correlation among material composition, processing conditions, and composite performance is mostly nonlinear. This level of complexity aligns with the heterogeneous interactions that have been reported with graphene-reinforced systems of cementitious materials (Lin & Du, 2020; Suo et al., 2020).

The mechanical strength of the GNP-, GO-, and rGO-modified composites differed, with the rGO-containing composites showing a mildly higher mean UCS. Graphitic materials have the ability to enhance cementitious performance by refining microstructures, nucleating, bridging cracks, and altering hydration products. Their efficacy, however, is highly dependent on dosage, morphology and dispersion. The same experimental results in the past prove that graphene oxide can modify the mechanical and microstructural behavior of concrete (Akarsh et al., 2021; Kedir et al., 2023). The fact that graphene-based cement materials are supported by broader developments also promotes their ability to be high-performance modifiers (M. Han et al., 2021).

Significant variations in ER were found among the graphitic-materials, GNPs composites had lower average resistivity than GO and rGO composites. This tendency states that graphitic properties determine the development and maintenance of conductive channels in the cement matrix. Carbonaceous substances have the potential to form electrically responsive networks under the right dispersion and concentration regimes, which is the core of self-sensing cementitious composites (Bekzhanova et al., 2021; J. Han et al., 2020). Graphene-based conductive networks can thus be especially useful for next-generation smart concrete systems (W. Li et al., 2022).

Tree-based models have shown higher performance compared to all conventional Linear Regression models in general, indicating the significance of nonlinear interactions among material variables. Random Forest offered UCS reliable generalization and Decision Tree Regression yielded the best ER prediction. The same benefits of nonlinear machine-learning methods have been observed in concrete strength prediction, especially when the characteristics of the mixtures interact in a complex manner (Malhotra et al., 2023; Nguyen et al., 2022). The relatively poor performance of the Linear Regression also indicates that simple additive relationships are not sufficient to model these material systems.

The feature-importance analysis revealed curing age, water-to-cement ratio, graphitic thickness, and ultrasonication to be important predictors of UCS. On the other hand, graphitic content, water-to-cement ratio, AD, graphitic surface area, and use of superplasticizer were specifically effective in ER. The findings have physical plausibility since the dosage and surface characteristics of graphitic materials influence the interaction of the particles, dispersion, hydration and formation of a conductive network. Ongoing studies also highlight that the dosage and material properties of graphene oxide significantly influence the functionality of cement composites (Bagheri et al., 2022; Zeng et al., 2023).

The high predictive success achieved in the work is in line with the growing use of machine learning in the characterization of cementitious materials. Past studies have shown that XGBoost can effectively model the compressive strength of concrete whereas explainable machine-learning models can provide insight into the variables being modeled by otherwise black-box models (Ekanayake et al., 2022; Nguyen et al., 2022). The current results build on this idea based on the structural and electrical response in graphitic-material-modified composites.

The models created can be used to optimize materials in preliminary stages prior to carrying out a large-scale experimental procedure. Precise prediction of UCS and ER can minimize laboratory trials, material use, cost and development time and help in choosing the graphitic dosage and processing conditions. These features are especially useful in multifunctional and self-sensing concrete projects that need a combination of structural stability and electrical responsiveness (Bekzhanova et al., 2021; W. Li et al., 2022).

The analysis was based on data, and some of the graphitic-material properties, especially the surface area, had significant amounts of missingness. In addition, UCS and ER were recorded in different datasets and were not specimen-matchable. Future studies ought to utilize larger, externally validated experimental datasets with paired mechanical and electrical measurements. Additional model validation via experimentation and broader material characterization enhance model generalizability and enable the establishment of an optimized graphene-based cementitious composite.

5. Conclusion

The present study has shown that data-driven machine-learning methods can be effective in predicting the mechanical strength and electrical resistivity of graphite-modified cementitious composites. Different predictive models were created for unconfined compressive strength and electrical resistivity since the two outputs were in independent data sets. Random Forest was the best performing model in the prediction of UCS, with an R2 of 0.888, and Decision Tree Regression was the best model in predicting electrical resistivity, with an R2 of 0.991. The feature-importance analysis further revealed that mechanical strength was sensitive to curing age, water-to-cement ratio, graphitic-material thickness, and ultrasonication but resistivity was sensitive to the graphitic content, water-to-cement ratio, surface area, use of superplasticizers and other conditions related to electrical measurements. These results suggest that mechanical and electrical characteristics of graphite-modified cementitious materials are controlled by various and yet related material and processing factors. The findings also support the fact that nonlinear machine-learning models are more adequate compared to the traditional linear methods to capture these complex relationships. Altogether, the suggested predictive framework has the potential to facilitate more effective design of materials, minimize experimentation load and help to create multifunctional and self-sensing cementitious composites. The models should be proven by future studies on large external datasets under paired mechanical and electrical measurements.

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