Microstructural Analysis and Machine Learning-Based Prediction of Polymer-Modified Soil Characteristics

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ABSTRACT

The use of polymers in geotechnical engineering has accelerated rapidly due to their ability to enhance the mechanical and physical properties of soils. However, despite increasing interest, predicting the behavior of such materials across varying polymer concentrations remains a challenge and requires additional tools for an accurate evaluation. This study presents an integrated approach to the analysis and prediction of microstructural changes in polymer-modified soils that combines microscopy techniques with machine learning methods. A detailed microstructural analysis was conducted on soils modified with Xanthan Gum (XG) and Carboxymethyl Cellulose (CMC) using Scanning Electron Microscopy (SEM), Energy-Dispersive X-ray Spectroscopy (EDS), and elemental and morphological heatmap visualizations. These techniques allowed for a comprehensive investigation of microlevel changes occurring due to varying polymer concentrations. Based on experimental data, a linear regression model was developed to predict microstructural characteristics at a polymer concentration of 12%, an untested level in the laboratory. The results show that machine learning-based predictions derived from experimental data at lower concentrations (3%, 6%, and 9%) can effectively estimate microstructural parameters at higher concentrations. This approach offers a cost-effective and time-saving solution for the development of new and sustainable soil modification strategies. The optimized soil-to-polymer ratio is key to consistent microstructural modification.

Keywords-polymer; soil; microstructural analysis; machine learning; morphology

I. INTRODUCTION

Weak soils are unable to withstand significant loads without deformation [1]. Construction on such soil leads to the settlement of the foundation and uneven deformation of structures. Stabilization of weak soils is essential to ensure the stability of engineering structures and prevent adverse outcomes [2]. This procedure is particularly important in construction projects carried out in areas with problematic engineering and geological conditions [3]. Methods of soil

improvement include the replacement of weak soil with more stable material and the use of pile foundations, which transfer loads to deeper and denser layers [4]. In certain cases, chemical stabilization or mechanical compaction is applied to enhance soil properties [5]. One of the promising approaches involves the use of biopolymers for soil stabilization [6]. Biopolymers provide an environmentally friendly alternative to conventional chemical stabilizers. In addition, biopolymers are biodegradable, contributing to the ecological sustainability of stabilized soil.

The analysis of microstructural changes resulting from soil modification plays a key role in evaluating stabilization processes. This practice provides deeper insight into the underlying strengthening mechanisms and allows an objective assessment of the effectiveness of the treatment. In [7], the influence of microstructural parameters on the strength development of cement-stabilized marine clay was investigated, using Scanning Electron Microscopy (SEM) and a pore/crack analysis system to examine how the microstructure of the samples affects their unconfined compressive strength. Particular attention was given to parameters such as porosity, particle shape, size, and arrangement. Based on the data obtained, an exponential relationship was identified between microstructural characteristics and strength performance. In [8], nanoparticles were used to enhance the durability and strength of cement-treated soils in harsh marine environments. Among the materials tested, Nano-SiO_2 showed the most significant improvement, increasing strength by more than three times and reducing corrosion by 85% after repeated exposure to seawater. Results on the treatment of sandy soils using a novel zein biopolymer showed that even a small amount of zein significantly improves soil strength and elasticity, with performance increasing with time and with a higher binder content [9]. Microscopic analysis revealed that the protein network of zein enhances interparticle bonding through electrosteric stabilization, especially in soils with a wide grain size distribution and higher dry density. Microstructural analyses of soils modified with biopolymers, such as Xanthan Gum (XG) [10], chitosan [11], agar [12], starch [13], and guar gum [14], have demonstrated their effectiveness in improving the structure and enhancing interparticle bonding.

Despite the large number of studies focused on biopolymer-based soil modification, approaches to the composition design of polymer-modified soils beyond experimental methods remain limited and underexplored. This study aims to fill this gap by integrating microstructural analysis with machine learning techniques for predictive modeling at untested polymer concentrations, offering a data-driven tool to optimize soil treatment strategies without extensive laboratory testing.

II. MATERIALS AND METHODS

Soil from Astana, Kazakhstan, was used for the experiment. A sieve and an areometer analysis and liquid and plastic limit tests were performed to classify the soil [15]. Table I presents the physical characteristics of the soil tested. According to GOST 25100-2020 [16], the soil was sandy clay loam. XG and Carboxymethyl Cellulose (CMC) were used as soil modifiers. XG is a microbial exopolysaccharide synthesized by Xanthomonas campestris, characterized by its high viscosity and the ability to form stable gel-like structures in aqueous solutions [16]. CMC is a cellulose derivative containing anionic functional groups that provide good water solubility and the ability to interact with the mineral components of the soil.

TABLE I. SOIL CHARACTERISTICS

Soil characteristic	Value
Specific gravity, kg/m^3	2671
Maximum dry density, kg/m^3	1547
Optimum water content, %	9.605
Sand fraction (2.00 - 0.05 mm)	22%
Silt fraction (0.05 - 0.002 mm)	33%
Clay fraction (<0.002 mm)	45%
Liquid limit, WL, %	19.357
Plastic limit, WP, %	3.170
Plasticity index, Ip, %	16.187

Biopolymer solutions of XG and CMC biopolymer solutions were prepared at concentrations of 3%, 6%, and 9% by weight relative to 100 g of oven-dried soil. Accordingly, 3, 6, and 9 g of each biopolymer were dissolved in 20 g of distilled water. The 3% concentration was selected as a typical value frequently reported in the literature, while the 6% and 9% concentrations were included to expand the dosage range and assess the effects of higher biopolymer content on the microstructural behavior of the soil. This approach allowed detailed analysis of particle aggregation, internal structure formation, and saturation of microstructural changes induced by biopolymer treatment. The resulting dataset also supports the development of predictive models at a wider range of concentration levels, including those less explored in previous studies.

The solutions were prepared using the wet mixing method to ensure uniform dispersion of the biopolymer in the solution before applying it to the soil. The wet mixing technique facilitates complete dissolution and homogeneous distribution of the biopolymers, preventing clumping and ensuring optimal interaction with the soil matrix.

A. Microstructural Analysis Using Scanning Electron Microscopy (SEM)

To observe surface morphology and structural changes caused by biopolymer modification, SEM visualization was carried out using a Hitachi TM4000Plus scanning electron microscope in ENU-Lab. High-resolution images were obtained to assess the particle arrangement, their aggregation, and the formation of new structures within the soil matrix. SEM images were used as the basis for further quantitative analysis.

B. X-Ray Spectroscopy (EDS) Analysis

To determine the chemical composition of the modified and unmodified soil samples, Energy-Dispersive X-ray Spectroscopy (EDS) analysis was performed using a Hitachi TM4000Plus scanning electron microscope equipped with an EDS detector. Analysis was performed on selected regions of the sample surface to obtain point spectra and elemental distribution maps. Quantitative and qualitative data on the elemental composition were collected for further processing.

Based on the obtained EDS data, an elemental heatmap was generated to visualize spatial variations in the concentration of chemical elements. Data processing and visualization were carried out using Python, employing standard scientific libraries such as NumPy, Pandas, and Matplotlib. This approach allowed flexible data handling and a clear graphical representation of elemental distribution patterns.

C. C Quantitative Analysis of Soil Particle Morphology Using SEM Imaging

Quantitative analysis of SEM images of unmodified and modified soil samples was performed using CellProfiler, an open-source software designed for high-throughput image analysis. The key morphological parameters selected for comparison included area, which quantifies the surface coverage of individual particles, equivalent diameter, representing the diameter of a circle with the same area as the particle, eccentricity, which indicates the degree of elongation or deviation from circularity of the particles, solidity, reflecting the proportion of the particle's area to its convex hull, and form factor, which provides a measure of the particle's shape complexity. These parameters were used to evaluate the effects of biopolymer modification on soil particle morphology and the formation of new structures within the soil matrix.

D. Particle Distribution Heatmap Generation

The Fiji program (ImageJ) was used to visualize the spatial distribution of particles in SEM images of unmodified and modified soil. The construction of heat maps showing the particle density in different regions of the image included the following steps: image conversion to 8-bit format, application of a Gaussian filter to improve the quality of analysis, and construction of a histogram based on the image.

E. Development of a Machine Learning Model for Predicting Microstructural Characteristics

A machine learning model using Python 3.11.6 was developed to predict the microstructural characteristics of biopolymer-modified soil in a different concentration range (at 12% concentration). The model was trained on data obtained at sample concentrations of 0, 3, 6, and 9% to predict microstructural changes at the new concentration. A separate linear regression model was trained for each morphometric characteristic. Each model used polymer concentration as an input parameter and predicted the corresponding value of the characteristic. During data processing, Pandas 2.2.2, NumPy 1.26.4, and scikit-learn 1.4.2 libraries were used to organize and process tabular data, perform numerical calculations, handle array operations, and develop linear regression models to predict soil morphology characteristics. The Leave-One-Out Cross-Validation (LOO-CV) method was used to evaluate the predictive performance of the model. The Absolute Error (Abs Error) between the predicted and actual values was calculated only for the CMC12 data to verify the model's performance. Linear regression was selected for its simplicity, interpretability, and suitability for the type of data used in this study. Moreover, the limited number of data points, typical of laboratory-scale testing, favors models such as linear regression, which are less prone to overfitting and provide clearer insight into the influence of input parameters.

III. RESULTS AND DISCUSSIONS

A. SEM Results

Figure 1 presents SEM images of the surface structure of soil samples. A comparative analysis indicates that the morphology of polymer-modified soils varies not only with polymer type (XG vs. CMC) but also with concentration. Control samples show a porous structure, but biopolymer-treated samples reveal aggregation and binding, indicating improved integrity.

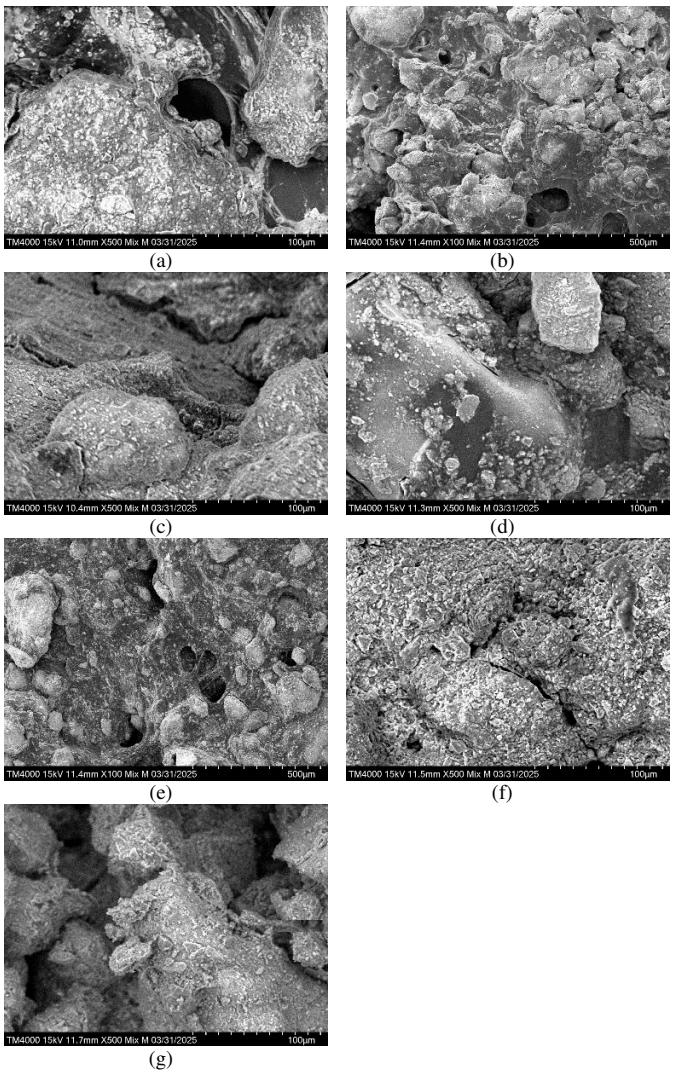

Fig. 1. SEM images of soil: (a) XG3, (b) XG6, (c) XG9, (d) CMC3, (e) CMC6, (f) CMC0, (g) US.

B. EDS Results

Figure 2 shows the heat map, which reflects the variation of the element concentrations between the control and the modified soil. The heat map visually highlights areas with the largest changes.

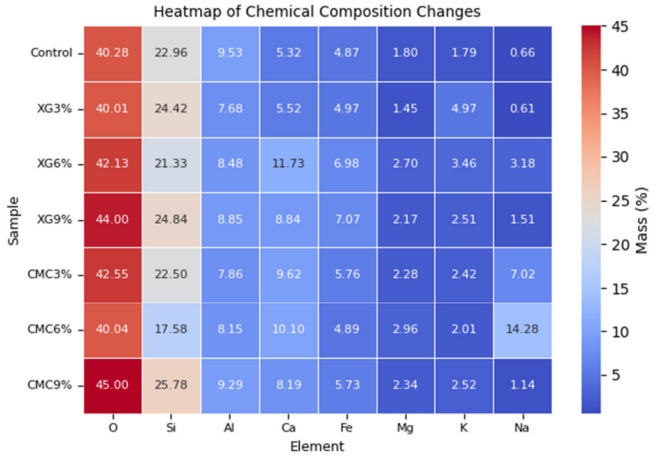

Fig. 2. Elemental heatmap visualizations.

Carboxymethyl cellulose is used in the form of a sodium salt ($Na-CMC$), which is capable of undergoing ion exchange reactions with soil cations such as Ca^{2+} and Mg^{2+} (1). This explains the substantial increase in sodium (Na) concentration observed in the CMC 6% sample, as shown in Figure 2, where the content rises from 0.66% in the control to 14.28%.

$$2CMC-COONa + Ca^{2+} \rightleftarrows (CMC-COO)_2Ca + 2Na^{+} \quad (1)$$

Biopolymers contain functional groups such as carboxyl ($-COO^{-}$) and hydroxyl ($-OH$), which are capable of coordinating with multivalent cations such as Fe^{3+}, Al^{3+}, and Ca^{2+}, as illustrated in (2-4).

$$Fe^{3+} + 3\,CMC-COO^{-} \rightarrow [Fe(CMC-COO)_3] \quad (2)$$

$$Al^{3+} + 3\,CMC-OH \rightarrow [Al\,(OH-CMC)_3] \quad (3)$$

$$Ca^{2+} + 2\,XG-COO^{-} \rightarrow (XG-COO)_2Ca \quad (4)$$

Such reactions contribute to the binding and stabilization of cations within the soil matrix, as evidenced by the increased concentrations of Fe (from 4.87% in the control to 7.07% in XG9%), Ca (from 5.32% to 11.73% in XG6%), and Mg (from 1.80% to 2.96% in CMC6%).

Monovalent cations (K^{+}) can form relatively weak coordination interactions with functional groups within the polysaccharide matrix, contributing to temporary binding and redistribution within the soil structure (5).

$$XG-COO^{-} + K^{+} \rightleftarrows XG-COOK \quad (5)$$

The increase in potassium concentration in the XG-modified samples (up to 4.97% in XG 3%) supports this mechanism. These chemical equations demonstrate that the interaction between biopolymers and soil is not limited to the physical reinforcement of the structure but involves a wide range of chemical processes, including ion exchange, complex formation, and sorption. These processes contribute to ion immobilization and enhance structural stability.

C. SEM Analysis Results of Soil Particle Morphology

Soil particle morphology analysis showed that the particle area of the modified soil samples varies from 300.50 for CMC3 to 394.07 for XG3, while this value in the control samples is 303.52 (Figure 3). The changes in particle area indicate that the modification process promotes an increase in particle size, as observed in the XG3 and CMC9 samples, where areas are significantly higher compared to the control samples.

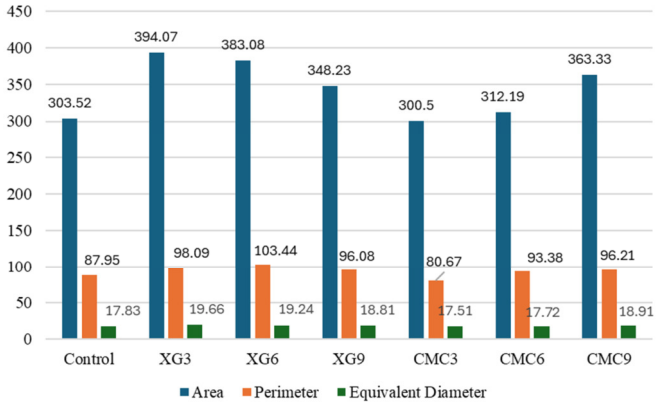

Fig. 3. Variation in Area, Perimeter, and Equivalent Diameter of soil particles in samples.

The perimeter of the particles in the control samples is 87.95 and ranged from 80.67 to 103.44 in the modified samples, with CMC3 showing a slight decrease, indicating a more rounded particle shape. The equivalent diameter, which characterizes the particle size, is 17.83 in the control samples and varied to 19.66 (XG3) in the modified samples. This increase indicates that the modification leads to an increase in particle size. The FormFactor is 0.49 in the control samples and ranges from 0.47 to 0.56 in the modified samples (Figure 4).

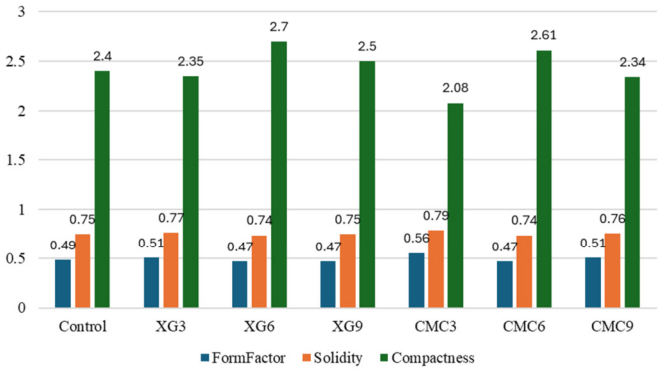

Fig. 4. Variation in FormFactor, Solidity, and Compactness of modified and control soil samples.

The increase in the FormFactor in CMC3, reaching 0.56, indicates the greater presence of particles with a more uniform and less elongated shape. The particle solidity for the control samples is 0.75. In most modified samples, this parameter ranges from 0.74 to 0.79, indicating stability. Particle compactness in the control samples was 2.40, while in the

modified soils it varied from 2.08 (CMC3) to 2.70 (XG6). This trend reflects a shift toward denser microstructural packing, particularly with XG, suggesting enhanced mechanical interlocking and reduced pore space.

D. Heatmap-Based Evaluation of Soil Particle Dispersion

Heat maps generated from SEM images of the modified soil exhibit a more uniform distribution of particle density across the entire image field (Figure 5).

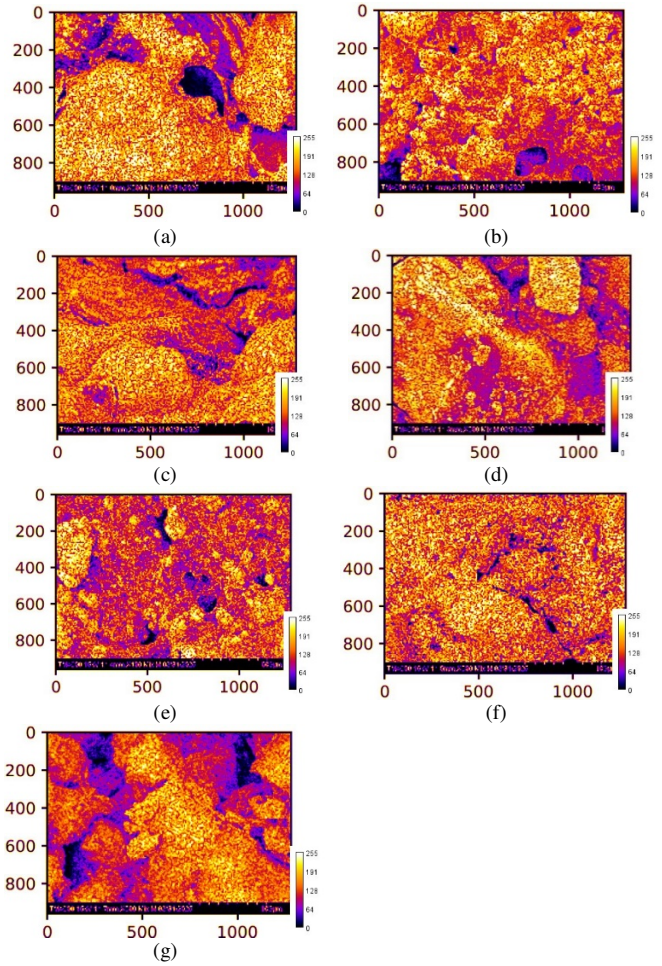

Fig. 5. Heatmap of soil particle dispersion: (a) XG3, (b) XG6, (c) XG9, (d) CMC3, e) CMC6, (f) CMC0, (g) US.

This indicates an increase in microstructural homogeneity and a reduction in porosity due to modification. In certain areas, a localized increase in particle density is observed, suggesting particle aggregation induced by the modifying agent, with this effect being particularly pronounced when XG is used (Figure 5 b and c). Higher polymer concentrations correspond to intensified particle clustering in heatmap images, indicating stronger interparticle interactions and reduced pore space. This compaction is attributed to the formation of polymer bridges that enhance the interparticle bonding and improve the overall integrity of the soil matrix. In contrast, the heat maps of the unmodified soil reveal a distinctly heterogeneous particle distribution, characterized by extensive low-density areas (Figure 5g). These areas indicate the presence of voids, high porosity, and weak interparticle interactions.

E. Model Performance and Prediction Outcomes

The predicted values (for the 12% XG, CMC concentration, with no experimental measurements) include key parameters such as area, perimeter, major and minor axis lengths, eccentricity, solidity, compactness, maximum radius, and equivalent diameter. Tables II and III summarize the results, and Table IV presents the predictions and calculated errors.

TABLE II. PREDICTED MICROSTRUCTURAL CHARACTERISTICS FOR XG 12%

Parameter	Predicted XG 12%	Observed trend	Interpretation
Area	388.01	Increase to XG3	Value higher than XG9
Perimeter	103.83	Gradual increase	Predicted value consistent with established trend
FormFactor	0.46	Minor fluctuations	Predicted value consistent with established trend
Solidity	0.745	Slight fluctuations	Within typical variability
Compactness	2.65	Irregular trend	Value within the observed range
Equivalent diameter	19.52	Increase to XG3, then decline	Aligned with the previously established trend

TABLE III. PREDICTED MICROSTRUCTURAL CHARACTERISTICS FOR CMC 12%

Parameter	Predicted CMC 12%	Observed trend	Interpretation
Area	367.66	Gradual increase	Value for CMC12 continues upward
Perimeter	98.92	Gradual increase	Perimeter increases consistently, and the trend remains stable.
FormFactor	0.50	Fluctuates	Minor fluctuations
Solidity	0.76	Slight decrease, then increase	Stable behavior
Compactness	2.44	Fluctuates	The predicted value suggests continued fluctuation.
Equivalent diameter	18.86	Gradual increase	CMC12 continues the increasing trend

TABLE IV. ABS ERROR FOR CMC 12%

Parameter	Actual	Predicted	Abs Error
Area	367.66	367.665	0.005
Perimeter	98.92	98.925	0.005
Equivalent diameter	18.86	18.855	0.005
FormFactor	0.50	0.500	~0
Solidity	0.76	0.755	0.005
Compactness	2.44	2.445	0.005

This is especially noticeable for the FormFactor parameter, where the absolute error was 0, signifying a complete match between the real and predicted values. In addition, a similar evaluation was performed for the 12% concentration of XG (XG12). The predicted values closely matched the actual measurements, with absolute errors ranging from 0 to 0.005. The perimeter and equivalent diameter showed deviations of 0.005. The application of the LOO-CV method helped reduce the risk of overfitting associated with the limited dataset. The

exclusion of one concentration level from the training process and its use as an unseen test sample confirmed the model's ability to generalize and accurately predict microstructural characteristics.

The results obtained in this study indicate that increasing the concentration of biopolymers exerts a significant influence on the microstructure of the modified soil, particularly affecting particle compactness, morphological characteristics, and overall structural densification. A comparative evaluation demonstrates that polymer concentration is the key parameter influencing microstructural evolution, while the type of biopolymer can be selected according to specific engineering requirements. The observed increase in morphometric indicators with concentration confirms the role of biopolymers in promoting soil matrix cohesion and particle organization [17]. These findings are consistent with previous studies [18].

Future studies may involve larger and more diverse datasets to improve model robustness and applicability, including combined soil treatments and a wider range of biopolymer types and concentrations. Techniques such as microcomputed tomography and Fourier-transform infrared spectroscopy could offer deeper insight into biopolymer-soil interactions compared to conventional methods such as SEM and EDS, although application is often limited by high cost, complex sample preparation, and the requirement for specialized equipment.

IV. CONCLUSIONS

The findings of this study confirm that the type and concentration of biopolymers have a pronounced effect on the microstructural characteristics of treated soils. In this study, XG6 exhibited higher compactness (2.70) and larger particle area, indicating its potential to form denser soil structures. In contrast, CMC3 demonstrated higher FormFactor (0.56) and Solidity (0.79), reflecting more symmetrical and stable structures under moderate loads and applying to conditions where uniformity and consistency are prioritized. Therefore, the selection of biopolymer type and concentration should be strategically aligned with the specific objectives of soil stabilization.

Furthermore, the machine learning-based prediction approach used in this study proved effective. The model accurately estimated microstructural parameters at higher concentrations based on data from lower concentrations. This approach is particularly beneficial when dealing with many experimental conditions, as it enables rapid estimation of key microstructural parameters, thereby accelerating the development of sustainable soil-modification strategies.

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