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Machine Learning-Based Constitutive Models for Soil-Water Retention, Hydraulic Conductivity, and Shear Strength of Unsaturated Saprolitic Soils

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Abstract

The mechanics of unsaturated soils is a relatively recent and evolving field of study. This paper introduces an innovative machine learning-based approach for developing constitutive models to describe the soil-water retention curve, hydraulic conductivity, and shear strength of unsaturated soils. These models were built using comprehensive soil characterization data and triaxial test results, incorporating parameters such as gravel, sand, silt, and clay content, plasticity index, porosity, and permeability. Equations were implemented using algorithms developed in the Mathematica® programming environment. The results demonstrate that the proposed models are both physically consistent and experimentally validated, exhibiting high precision and practical applicability. While this approach significantly optimizes the development of constitutive models, it does not replace the need for conventional testing, instead serving as a robust complementary tool. The proposed methodology offers an efficient and reliable solution for generalizing constitutive models across various unsaturated soil types, advancing knowledge and applications in the field.

Keywords

Unsaturated Soils, Machine Learning, Constitutive Models, Soil-Water Retention Curve, Hydraulic and Mechanical Behavior

1. Introduction

Classical soil mechanics provides a well-established framework for understanding the relationship between effective stress and shear strength. However, the behavior of unsaturated soils remains a topic of considerable debate. Traditional soil mechanics emerged primarily from studies of temperate climates and sedimentary soils, where the soil is typically regarded as a biphasic system composed of solid particles and water.

In tropical regions, such as the case examined in this study, environmental conditions promote the formation of thicker soil profiles, including mature residual soils and less developed young soils. Classical soil mechanics, therefore, does not fully account for the transitional nature of materials like young soils and saprolites. These materials occupy an intermediate phase between residual soils and intact rock, exhibiting properties that combine soil-like behavior with characteristics of weathered soft rocks. Such complexities suggest that classical soil mechanics may not provide a completely accurate representation of these transitional materials.

Understanding the mechanical and hydraulic behavior of transitional materials—ranging from poorly to highly developed soils derived from soft or altered rocks—is of critical importance. This behavior is strongly influenced by climatic variables, such as seasonal moisture fluctuations, and internal moisture variations caused by changes in the water table or other external factors. Additionally, the susceptibility of the parent rock to weathering cycles plays a significant role in these processes.

A key factor governing the mechanical and hydraulic behavior of unsaturated materials, particularly young soils, is the development of negative pore-water pressures (suction). Many natural destabilization processes are triggered by the reduction of suction, often caused by saturation resulting from various environmental conditions. As highlighted by Lopes (2006), the study of shear strength in unsaturated soils must incorporate the effects of suction. Furthermore, the unsaturated condition modifies the stress state, necessitating consideration of stress variables such as the net normal stress (σn-ua) and matric suction (ua-uw).

According to Silva (2011), the hydrological regime's influence operates on a local scale, where landscape elements such as altitude, slope angle, slope length and shape, and sun exposure must be accounted for. It is essential to acknowledge that geometry and morphology play critical roles in controlling surface and subsurface water flow, with geometry governing flow behavior in both saturated and unsaturated soil layers.

Campos et al. (2020) presented a model demonstrating that geometry significantly influences the distribution of pore pressures. Their findings revealed that concave shapes concentrate flow lines and elevate the water table, leading to increased pore pressure values. Similarly, Vilar (2021) emphasizes the necessity of updating or refining existing concepts to enhance the modeling of unsaturated soil behavior. This refinement is particularly important for improving predictive capabilities in routine geotechnical applications.

Das (2019) explains that water flow within the soil is driven by variations in the energy gradient and occurs through soil voids, provided sufficient continuity exists. Accurately representing flow under unsaturated conditions requires reliable acquisition of hydraulic properties, particularly the soil-water retention curve and the unsaturated hydraulic conductivity function.

Costa (2022) suggests that when considering soil volumetric variation, the water retention curve, and the hydraulic conductivity curve under unsaturated conditions, these properties become mutable hydraulic parameters. This mutability enables the conceptualization of retention and hydraulic conductivity surfaces. Based on this concept, constitutive surface models can be proposed for unsaturated soils. Nevertheless, robust constitutive models are still required to represent the porous medium's properties and solve the governing equations for unsaturated flow within this medium.

The Geofluxo Group at the University of Brasília (Research Group on Innovations and Technologies Applied to Environmental Geotechnics) has produced state-of-the-art research in developing constitutive models, as well as analytical and numerical modeling, for accurately representing unsaturated soil behavior (Costa & Cavalcante, 2020, 2021a, 2021b; Cavalcante & Mascarenhas, 2021; Mascarenhas & Cavalcante, 2022).

This study aims to provide valuable insights into altered rocks (saprolites and residual soils) found in the Carajás Mining Complex, specifically decomposed mafic rocks, commonly referred to as Decomposed Mafic (DM) rocks.

2. Literature Review

Fredlund and Rahardjo (1993) highlight that studies involving unsaturated soils have been of interest to soil mechanics since its establishment as an engineering discipline. This interest is justified by the prevalence of engineering projects that involve unsaturated soils, such as embankments, dams, and slope stabilization. Furthermore, the unsaturated condition is widespread globally, with arid and semi-arid climates accounting for approximately 60% of the world's land area. In tropical regions, such as Brazil, prolonged dry periods are sufficient to cause significant soil desaturation.

An unsaturated soil can be defined as a system composed of three distinct phases: solids, water, and air. These components form a structure where the void spaces, or pores, can store both liquids and gases. Fredlund and Morgenstern (1977) introduced the concept of an additional independent phase, termed the "contractile membrane," which represents the air-water interface within the soil. This phase influences the interaction between the fluid phases and the solid matrix.

In certain cases, unsaturated soils may be considered biphasic systems, particularly when the pores contain water with occluded air bubbles that lack interconnectivity (Fredlund & Rahardjo, 1993). Under these conditions, assuming that fluids fully occupy the pore space can significantly alter the soil's mechanical and hydraulic behavior. **Figure 1** illustrates the phase model representation for unsaturated soils.

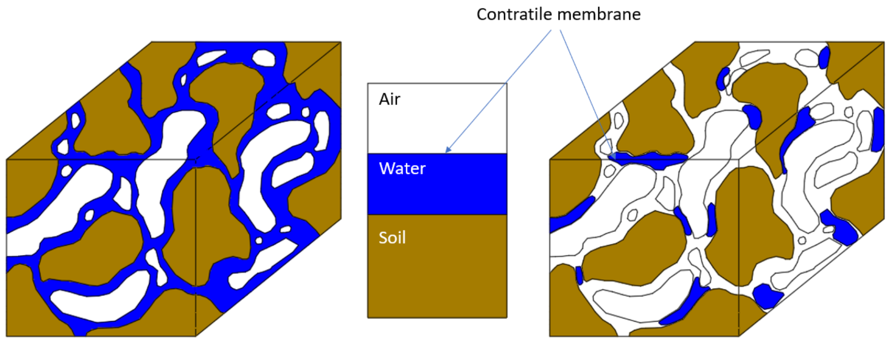

Figure 1. Phase diagram for unsaturated soils, showing the representation of the contractile membrane.

In unsaturated soils, negative pore-water pressure, commonly referred to as suction, significantly influences their mechanical behavior. Numerous studies have aimed to extend the concept of effective stress, originally introduced by Terzaghi (1936), to account for stress variations in unsaturated soils.

Bishop and Blight (1963) revisited the effective stress equation for unsaturated soils and observed that variations in matric suction (ua-uw) do not affect soil behavior in the same way as variations in net normal stress (σn-ua). To address this, they proposed a framework where net normal stress and matric suction are treated as independent stress variables. This concept is typically represented in three-dimensional plots, as illustrated in **Figure 2**.

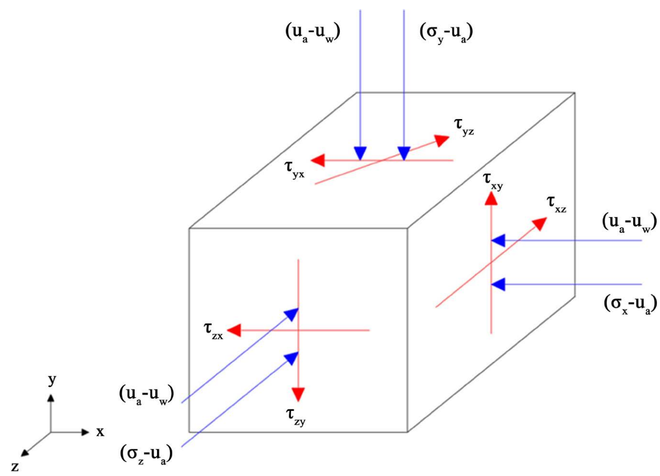

Figure 2. Three-dimensional representation of stress variables in unsaturated soils, showing net normal stress and matric suction as independent axes.

Fredlund et al. (1978) expanded on the earlier concepts by introducing two independent stress state variables: net normal stress (σ-ua) and matric suction (ua-uw), to describe the geomechanical behavior of unsaturated soils. These variables have since become widely accepted for defining the stress state in unsaturated soils. Suction plays a key role in water retention and significantly impacts the soil's ability to conduct water through its pores. One of the most effective tools for characterizing unsaturated soil behavior is the soil-water retention curve (SWRC).

The soil-water retention curve is fundamental for understanding the interaction between soil and water, particularly in unsaturated conditions. It graphically represents the relationship between moisture content and suction, illustrating the water content present within soil pores at varying suction levels. Key parameters derived from the SWRC include the air entry value—the critical suction at which water begins to drain from the largest pores—and the residual moisture content, which indicates the point at which moisture is no longer significantly reduced despite increasing suction (Gerscovich, 2001).

The shear strength of unsaturated soils is influenced by several factors, including density, soil structure, moisture content, and the proportion of fine particles. Generally, unsaturated soils demonstrate lower shear strength compared to saturated soils, as the presence of water enhances cohesion and increases the soil's load-bearing capacity.

Costa (2022) noted that existing models for the soil-water retention curve (SWRC) and hydraulic conductivity in unsaturated soils are primarily developed for soils with a unimodal pore distribution. However, authors such as Durner (1994) and Liu et al. (2013) emphasize that unimodal models fail to accurately capture the behavior of bimodal soils, which exhibit distinct air entry points in their retention curves.

Albuquerque et al. (2022) applied machine learning techniques to predict the soil-water retention curve using soil characterization parameters such as plasticity index and porosity. Their findings demonstrated that the proposed algorithm offers a viable and efficient alternative for estimating the SWRC, significantly improving the method's practicality and accuracy.

3. Case Study

3.1. Location

The study was carried out in an iron mine located in Brazil. This region is notable for its history of significant instability events and large-scale ruptures, making it an ideal site for studying the geomechanical behavior of unsaturated saprolitic and residual soils.

3.2. Characterization and General Context

The southwestern sector of the mine exhibits a complex geological sequence, predominantly composed of metavolcanic and sedimentary formations. The primary lithology consists of altered mafic rocks, including metabasalt and metadiabase, which have undergone varying degrees of weathering. This alteration process has led to the formation of thick layers of saprolitic materials, exhibiting clayey to silty textures with colors ranging from red to yellow and brown.

Locally, these rocks are classified based on their degree of weathering and strength into three categories: Fresh Mafic, Slightly Decomposed Mafic, and Decomposed Mafic. These materials demonstrate a pronounced tendency to lose strength rapidly when exposed to water or high humidity conditions.

The predominant lithological units in the region are decomposed mafic rocks, which exhibit poor geomechanical quality, classified as Class IV according to the modified Bieniawski classification.

3.3. Geotechnical Event and Motivation

The motivation for this study stems from a significant rupture event involving a 90-meter-high slope composed of altered soft rocks, specifically saprolites derived from mafic rocks. The slope exhibited varying degrees of alteration, which contributed to its instability. This geotechnical event was not isolated, as similar high and unstable slopes are widespread within the mine and other areas. These slopes share comparable geotechnical conditions and exhibit susceptibility to failures of similar magnitude.

During the slope recovery process, additional rupture events occurred, particularly at the bench level. These subsequent failures were primarily driven by increased saturation of the slope materials, which led to a significant reduction in the strength parameters of the mafic rocks. Figure 3 illustrates the historical timeline of instability events and failures, providing a comprehensive overview of the occurrences and their progression over time in the N5W Mine.

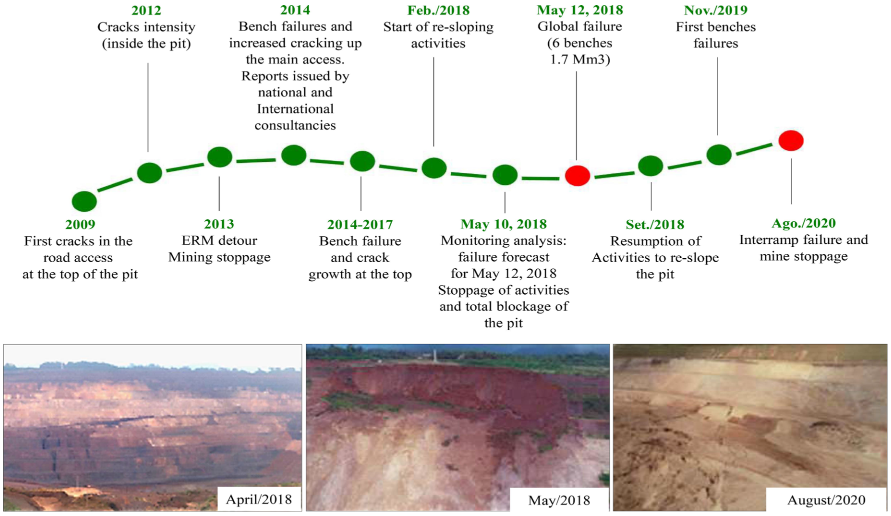

Figure 3. Historical timeline of instability events and failures.

This study aims to incorporate concepts from unsaturated soil mechanics to improve the understanding of these failure events and the underlying rupture mechanisms, providing insights that can aid in the assessment and stabilization of similar slopes in the region.

4. Methodology

For this study, deformed and undeformed soil samples of saprolitic/residual materials (decomposed mafic rocks) were collected for characterization and triaxial tests (CU Triaxial tests in both natural and saturated states).

The constitutive models for the soil-water retention curve and shear strength were initially determined using the machine learning technique proposed by Albuquerque et al. (2022).

The methodological approach utilized data from soil characterization tests, including gravel, sand, silt, and clay percentages, as well as the plasticity index and porosity, to derive parameters such as volumetric water content and total suction.

Soil physical characterization data (percentages of gravel, sand, silt, and clay, plasticity index, and porosity) were used to derive parameters such as volumetric water content and total suction. This data served as input for machine learning estimators developed in the Python programming language to predict the volumetric water content and suction behavior of the soil.

The methodology leverages the potential of machine learning techniques, including extremely randomized trees, random forest, decision trees, logistic regression, support vector machines, multi-layer perceptron, and k-nearest neighbors, to model the soil-water retention curve (SWRC) behavior for various soil types.

The preliminary database included 794 measured SWRC points (main drying branch), alongside corresponding soil characterization properties obtained from a diverse range of soils, as compiled by the authors. This dataset was divided into training, cross-validation, and test sets, which were used to fit, optimize, and evaluate the predictive models, respectively.

Subsequently, the functions proposed by Cavalcante and Zornberg (2017a), Cavalcante and Zornberg (2017b) and Costa and Cavalcante (2021a) were fitted to the machine learning predictions, generating a continuum function. This function can be utilized in other applications, such as numerical simulations and geotechnical modeling.

It is important to emphasize that machine learning models can be continuously updated by incorporating new training soil samples as additional data becomes available, including measured suction, volumetric water content, and corresponding characterization parameters.

The results demonstrate that the proposed machine learning estimator offers a promising alternative for estimating the soil-water retention curve (SWRC) in engineering practice.

This technique provided the basis for determining the preliminary analysis parameters. Subsequently, an algorithmic solution was implemented in the Wolfram Mathematica® software, utilizing the formulations proposed by Costa and Cavalcante (2020, 2021a, 2021b) and Cavalcante and Mascarenhas (2021). A streamlined representation of the adopted methodology is shown in **Figure 4**. The flowchart provides a structured and systematic approach to analyzing the geotechnical behavior of soils. The process begins with soil sampling, involving both deformed material and undeformed blocks. The collected samples are subjected to:

- Granulometric characterization,
- Permeability assessment, and

- Triaxial tests (CU saturated and CU natural states).

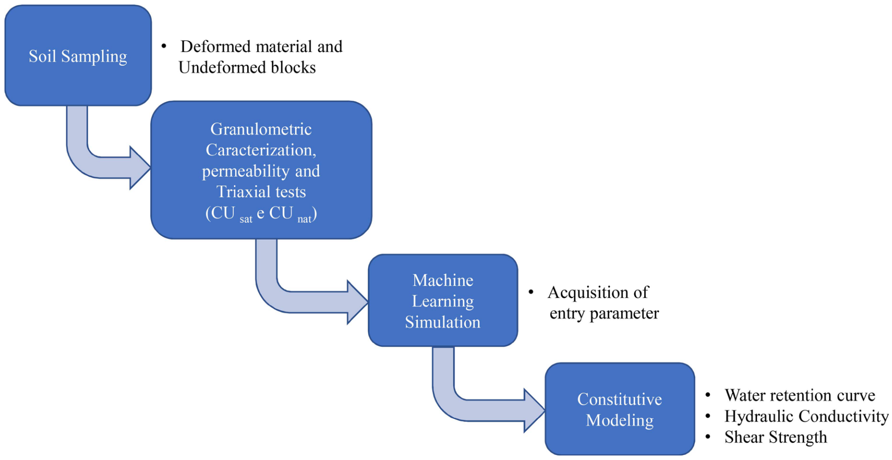

Figure 4. Flowchart of adopted methodology.

The results from these tests serve as input for machine learning simulations, which play a pivotal role in determining specific entry parameters. These parameters form the basis for constitutive modeling, where critical attributes such as the soil-water retention curve, unsaturated hydraulic conductivity, and shear strength are derived.

This comprehensive process facilitates a deeper understanding of the soil's geotechnical properties and behavior under various conditions.

Table 1 and Table 2 present the collected data and the parameters utilized in the simulation and modeling to predict the soil-water retention curve.

The potential of machine learning to predict the soil-water retention curve was explored by developing estimators in Python using the scikit-learn library. Additional tools that supported the process include pandas, NumPy, matplotlib, Jupyter Notebook and Anaconda Navigator.

An overview of the adopted methodology is illustrated in Figure 5, adapted from Scikit-learn. The figure represents a typical cross-validation workflow in model training. To develop and select the most appropriate machine learning model:

1) Training was performed on the training set,

2) Evaluation was conducted using the cross-validation set to fine-tune the model, and

3) Once the experiments indicated satisfactory results, the final evaluation was performed on the test set.

This systematic approach ensured the reliability and robustness of the predictive models for estimating the soil-water retention curve.

To mitigate overfitting, a standard practice in supervised machine learning experiments is to set aside a portion of the available data as a test set. In this study, 20% of the data (159 points) were reserved for testing.

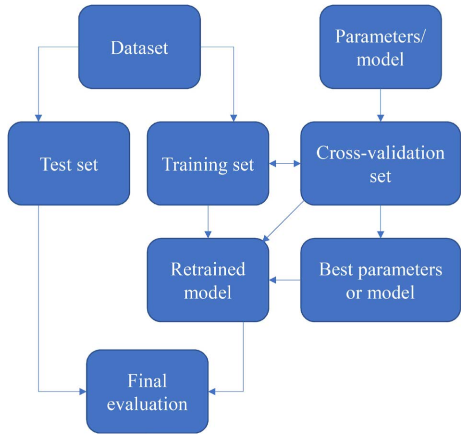

Figure 5. Flowchart of a typical cross-validation workflow.

The data were randomly divided into training and test sets using a stratified shuffle split. This method was employed because the majority of suction data falls within the range of 10^2 to 10^3 kPa. Stratified splitting ensures that each suction interval, as defined in Figure 6, maintains a proportional distribution of data points.

This approach enables a robust assessment of the generalization performance of the machine learning models across the entire suction range, ensuring accurate predictions for both high and low suction values.

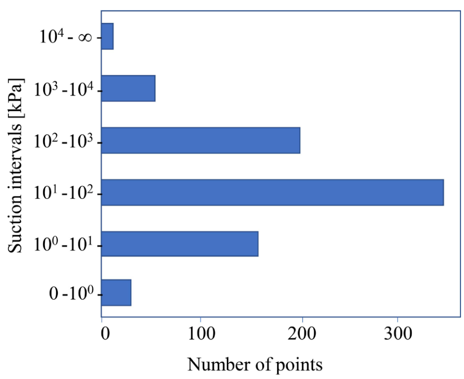

Figure 6. Suction intervals of the data test.

For most machine learning estimators, it is essential that the data are scaled and any missing values are addressed. Estimators can behave unpredictably if individual features do not approximate standard normally distributed data. To address this, the data were scaled using standardization, which involves removing the mean and scaling to unit variance.

Regarding missing data, only 1.4% of the sand and silt percentage values and 4.6% of the plasticity index values were absent. Since these were relatively small amounts, they were replaced with the mean value of each respective feature.

When comparing different estimators or adjusting hyperparameters, there remains a risk of overfitting on the test set, as performance on the test data can influence model selection or parameter tuning. Overfitting occurs when the test set indirectly informs the model, causing evaluation metrics to lose their reliability in assessing generalization performance.

To mitigate this, another subset of the data, known as the cross-validation set, was held out for model evaluation. A 5-fold cross-validation strategy was employed, where the dataset is split into five folds, and the model is trained and validated iteratively.

To optimize model performance, the hyperparameter space was systematically explored using grid search cross-validation. This method exhaustively evaluates all possible parameter combinations provided and identifies the best combination based on the cross-validation score.

As an example, some hyperparameters of a decision tree are as follows: min_samples_split, the minimum number of samples a node must have before it can be split; min_samples_leaf, the minimum number of samples a leaf node must have; and max_features, the maximum number of features evaluated for splitting at each node. Additionally, the hyperparameters n_estimators, random_state, and ccp_alpha control the number of decision trees in the ensemble, the randomness of the process, and the pruning of the trees, respectively. Increasing the values of min_samples_split, min_samples_leaf, or ccp_alpha, or reducing max_features, can help regularize the model.

The training process was divided into two phases. Phase 1 involved fitting various types of machine learning estimators, including logistic regression, multilayer perceptron with the Adam optimizer and different activation functions (ReLU, hyperbolic tangent, sigmoid, and identity), support vector machines with different kernels (linear, polynomial, radial basis function, and sigmoid), k-nearest neighbors, decision trees, random forests and extremely randomized trees (Extra Trees) using the default settings in Scikit-learn. Detailed information about each model can be found in Géron's book and the Scikit-learn User Guide.

In Phase 2, the best-performing algorithm from Phase 1 was selected for fine-tuning its hyperparameters using a grid search cross-validation approach. The algorithm selection was based on the root mean squared error (RMSE) and the coefficient of determination (R^2) evaluated through 5-fold cross-validation.

To facilitate the application of the predicted output results, soil water retention curve (SWRC) points were fitted using three different models. Cavalcante and Zornberg (2017a) proposed a model that considers a single fitting parameter for the SWRC. Their study analytically solved Richard's equation, which governs unsaturated flow through porous media, for a one-dimensional flow using a rigorous approach.

5. Results

5.1. Results from Laboratory Tests

Table 1 and **Table 2** present the collected data and parameters used in the simulation and modeling processes to estimate the soil water retention curve (SWRC).

Table 1. Summary of granulometric characterization data used to derive the parameters for the soil water retention curve.

Sample	Type of simulation	Granulometric Distribution				Porosity Index n	Plasticity Index IP
		Gravel	Sand	clay	Silt		
Block 3*	simulation	2	17	14	67	0.45	29
Block 3**	real	5	95	-	-	0.66	27
Block 4*	simulation	5	23	12	60	0.45	16
Block 4*	real	5	28	7	60	0.65	16
Block 4**	real	5	95	-	-	0.65	16

Table 2. Summary of soil water retention curve parameters obtained using the AI simulator proposed by Albuquerque et al. (2022).

Sample	Type of simulation	θ_s	θ_r	δ_1	δ_2	λ	R^2
Block 3*	simulation	0.45	0.16	0.0001	0.0109	0.497	0.992
Block 3**	real	0.66	0	0.0018	231.52	0.44	0.873
Block 4*	simulation	0.45	0.14	0.0010	0.0125	0.341	0.99
Block 4*	real	0.65	0.02	0.0187	267.57	0.722	0.966
Block 4**	real	0.65	0	0.0040	283.09	0.499	0.922

5.2. Estimation of the Soil-Water Retention Curve Using AI (Machine Learning)

Constitutive models play a fundamental role in soil mechanics by providing mathematical tools to describe and predict the behavior of unsaturated soils under varying environmental and mechanical conditions. Unlike saturated soils, unsaturated soils contain both water and air within their pore spaces, which significantly influences their mechanical and hydraulic properties. A key factor in this behavior is matric suction, defined as the negative pressure exerted by water within the soil pores. Matric suction directly affects soil strength, deformability, and permeability, making it a crucial parameter for analyzing and predicting the physical properties of unsaturated soils in response to moisture content variations.

The constitutive modeling of unsaturated soils has extensive applications, including slope stability analysis, foundation design, and water resource management. These models are indispensable for civil engineering projects, as they allow for accurate predictions of soil responses to external loads and environmental changes. This predictive capability ensures safer and more efficient designs, particularly in regions with unsaturated soil conditions.

The simulation conducted using Wolfram Mathematica®, based on the model developed by Costa and Cavalcante (2020, 2021a), proved effective in determining key parameters such as hydraulic conductivity and shear strength. The results highlight the practical applicability of these models in geotechnical engineering, providing reliable tools for addressing complex soil behavior in real-world scenarios.

5.3. Estimation of the Soil-Water Retention Curve Using AI (Machine Learning)

The innovative methodology proposed by Albuquerque et al. (2022) for estimating the soil-water retention curve (SWRC) leverages advanced artificial intelligence (AI) techniques, specifically machine learning algorithms implemented in Python. This approach enables precise estimation of volumetric water content (θ) and matric suction (ψ), which are critical parameters for characterizing the hydraulic behavior of soils.

The implementation of this methodology requires input data from physical characterization tests, including gravel, sand, silt, and clay percentages, as well as the plasticity index and porosity. Using these inputs, the AI-driven framework adjusts constitutive models such as van Genutchen (1980), Cavalcante & Zornberg (2017a), Cavalcante & Zornberg (2017b) for unimodal soils and the model proposed by Costa & Cavalcante (2021a) for bimodal soils.

This methodology represents a significant advancement in modeling soil hydraulic behavior, offering a robust and efficient foundation for geotechnical analysis and design. Accurate SWRC prediction is particularly crucial in geotechnical engineering applications, including slope stability assessments, foundation design, and water resource management.

The AI tool developed for this purpose is accessible through the Geofluxo Group's application page and is available online. The platform's intuitive interface, illustrated in **Figure 7**, enables users to input characterization data and obtain reliable SWRC estimates seamlessly. This enhances efficiency and accessibility for geotechnical professionals and researchers, streamlining the process of predicting soil-water retention curves with greater accuracy.

Using data collected from physical characterization tests, computational simulations were conducted to determine the volumetric water content (θ) and matric suction (ψ), along with other key parameters necessary for the application of analytical solutions. These parameters enabled the development of constitutive models for shear strength and hydraulic conductivity under unsaturated conditions.

Figure 8 and **Figure 9** present the most significant results obtained from the simulations of the soil-water retention curve (SWRC). Notably, these results are derived from a combination of experimental data and sensitivity analysis-based simulations. This hybrid approach facilitated the refinement of the retention curves by accounting for variations in soil porosity and plasticity index.

The refinement process is critical for ensuring the accuracy and relevance of the developed constitutive models. These refined models provide a robust foundation for application in geotechnical engineering studies and projects, enabling precise predictions of soil behavior under unsaturated conditions.

The simulation of the soil-water retention curve (SWRC) confirmed that the results derived from characterization tests align well with the plasticity index values. However, a discrepancy was noted between the experimental porosity data and the results generated by the simulator, resulting in deviations of the simulated curves from the expected test data.

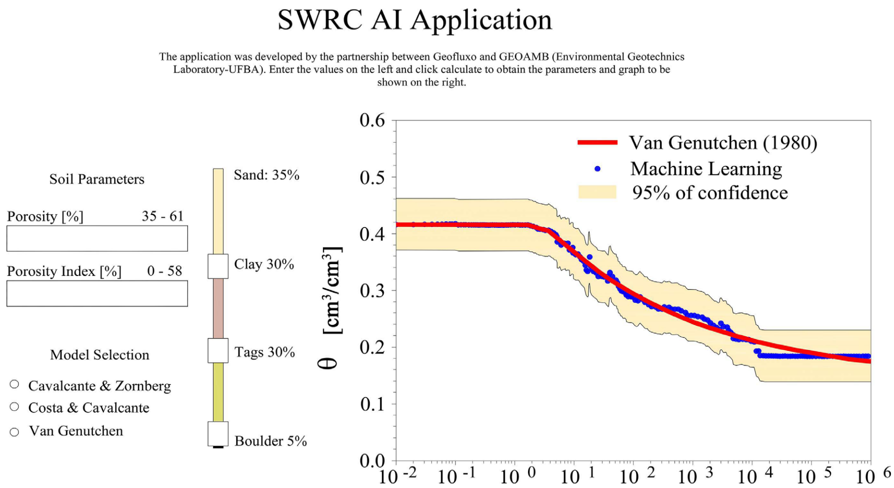

Figure 7. Artificial intelligence application page for obtaining the soil-water retention curve.

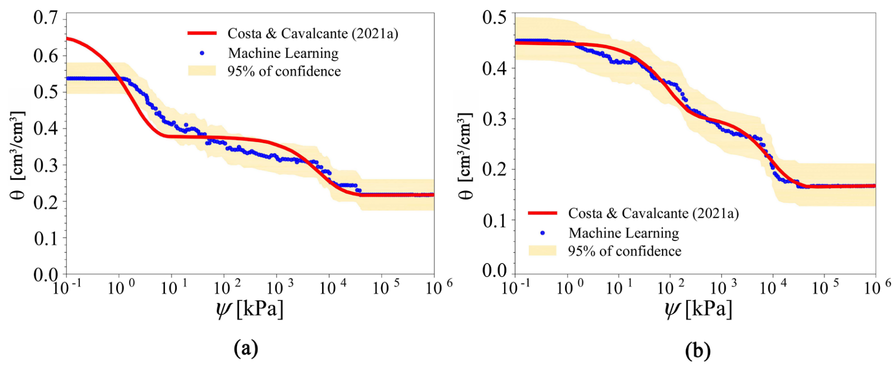

Figure 8. Soil-Water retention curve for Block 3. (a) Obtained from test data; (b) Sensitivity analysis for porosity to achieve a better curve fit.

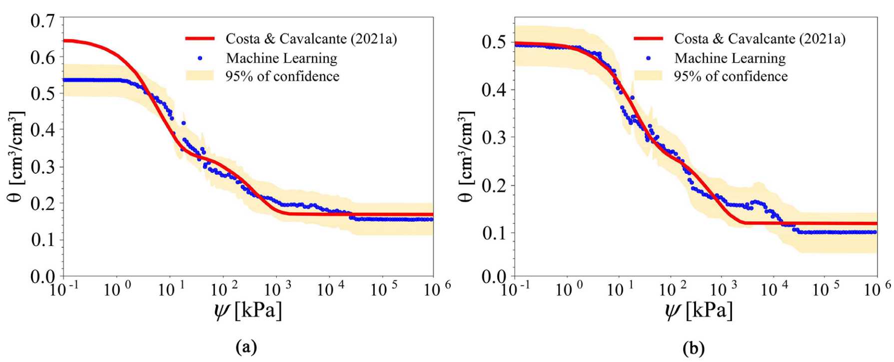

Figure 9. Soil-Water retention curve for Block 4. (a) Obtained from test data; (b) Sensitivity analysis for porosity to achieve a better curve fit.

The sensitivity analysis revealed that the porosity values most compatible with the simulated curves range between 41% and 48%. Despite these deviations, the curves obtained are considered acceptable for simulation purposes, as they provide a theoretical approximation of the soil behavior under unsaturated conditions.

It is essential to emphasize that the validation and calibration of the developed constitutive models must be performed using real data obtained from dedicated laboratory tests for the soil-water retention curve. This ensures the accuracy, reliability, and applicability of the models in geotechnical engineering projects.

5.4. Constitutive Model for the Soil-Water Retention Curve

The soil-water retention curve (SWRC) and unsaturated hydraulic conductivity are fundamental for determining soil states and conditions, which are critical for practical applications in geotechnical engineering. These properties provide insights into soil behavior under varying moisture conditions, enabling more precise analysis and design.

In recent studies, Costa and Cavalcante (2021a) and Costa (2022) introduced innovative models that focus on the hydraulic properties of bimodal soils, addressing the complexity of their retention behavior. These models represent a significant advancement, offering improved accuracy through the use of superimposed linear curves. Importantly, they achieve this with a limited number of fitting parameters, each with clear and well-established physical significance, enhancing both interpretability and usability for practitioners.

The model proposed by Cavalcante and Zornberg (2017a) laid the foundation for this research field, describing the relationship between volumetric water content (θ) and soil suction (ψ) through a specific mathematical expression. This precursor model serves as a basis for further developments, including the recent enhancements for bimodal soils.

$$\theta(\psi) = \theta_r + (\theta_s - \theta_r)\exp(-\delta|\psi|) \quad (1)$$

where:

θ is volumetric water content (L^3/L^3);

θ_s is the volumetric water content at saturation (L^3/L^3);

θ_r is the residual volumetric water content (L^3/L^3);

δ is the hydraulic adjustment parameter ($M^{-1}LT^2$);

ψ is the soil suction ($ML^{-1}T^{-2}$).

The advanced model proposed by Costa and Cavalcante (2020) is distinguished by its robust physical foundation, where each parameter is explicitly linked to the hydraulic properties and behavior of the soil. This model enables precise determination of the volumetric water content in both residual and saturated conditions through experimental methods.

A key aspect of the model is Equation (2), which establishes the direct relationship between the air-entry value (ψ_{ar}) and the hydraulic parameter (δ). This correlation is fundamental for understanding how physical variables influence water dynamics within the soil. By capturing these relationships, the model facilitates a deeper and more applied analysis of the soil's hydraulic properties under varying environmental and mechanical conditions.

$$\psi_{ar} = \frac{\exp\left(1-\exp(1)\right)}{\delta} \tag{2}$$

Adopting the linear superposition principle introduced by Costa and Cavalcante (2021a) and Costa (2022) enables the derivation of a bimodal model, as represented by Equation 20. This model marks a significant advancement in the study of soil hydraulic properties, offering a more precise and detailed description of soils exhibiting bimodal characteristics.

The linear superposition approach integrates two sets of characteristic curves—each corresponding to distinct porosity states within the soil—into a single, cohesive model. This integration allows for a comprehensive representation of the complex pore structure and water retention behavior unique to bimodal soils.

By capturing these intricate interactions, the proposed methodology enhances the understanding of soil behavior and serves as a robust predictive tool for analyzing soil hydraulic responses under varying environmental conditions. This advancement has practical implications for geotechnical engineering applications, particularly in scenarios where soils exhibit dual-porosity systems.

$$\theta(\psi) = \theta_r + (\theta_s - \theta_r)\left[\lambda \exp\left(-\delta_1|\psi|\right) + (1-\lambda)\exp\left(-\delta_2|\psi|\right)\right] \tag{3}$$

Using the previously discussed formulations and parameters extracted from the simulation of the soil-water retention curve (SWRC), a computational script was developed in Wolfram Mathematica®. This script was instrumental in the effective implementation of the proposed models, significantly streamlining the process of creating detailed constitutive models for soil-water interactions.

Through this computational approach, we accurately modeled and visualized the soil-water retention curves for various analysis blocks, ensuring high precision in the representation of hydraulic behavior. **Figure 10** and **Figure 11** present the modeled curves for Blocks 1, 3, and 4, respectively. These graphical representations provide critical insights into the hydraulic properties of the soils in each block, showcasing the models' applicability and accuracy in describing SWRC behavior. This computational methodology not only enhances the visualization of soil-water retention properties but also establishes a solid foundation for analyzing and understanding the complex interactions between water and soil under diverse conditions and scenarios. Such insights are invaluable for geotechnical engineering applications, improving the prediction and assessment of soil behavior in practical projects.

A detailed analysis of the graphs reveals a distinctly bimodal behavior in the soil-water retention curves, characterized by two well-defined plateaus or inflection points. This pattern is indicative of a bimodal pore distribution in the analyzed soils. The bimodal nature can be attributed to the presence of two distinct pore types:

- Macropores, which correspond to the void spaces between soil aggregates.
- Micropores, which are associated with voids within the aggregates themselves.

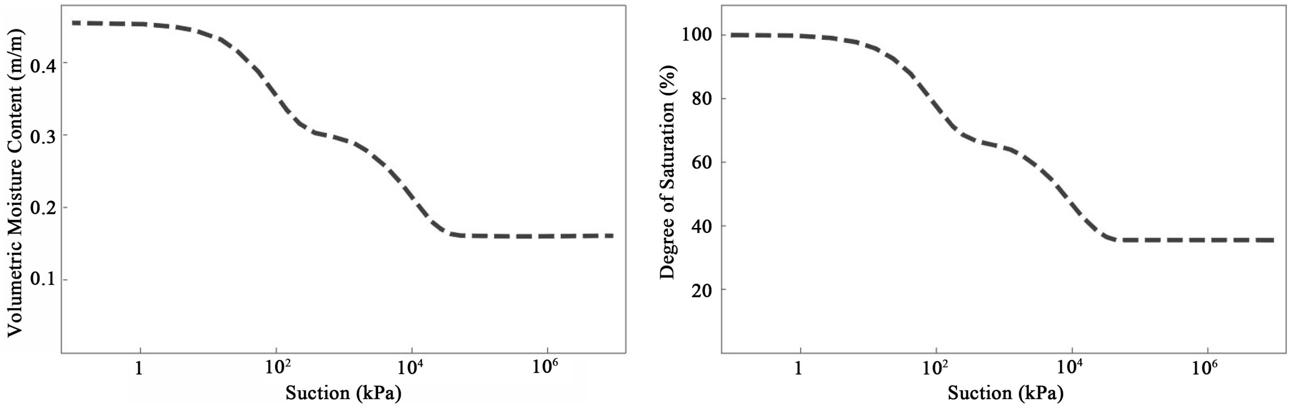

Figure 10. Soil-Water retention curve and degree of saturation for Block 3.

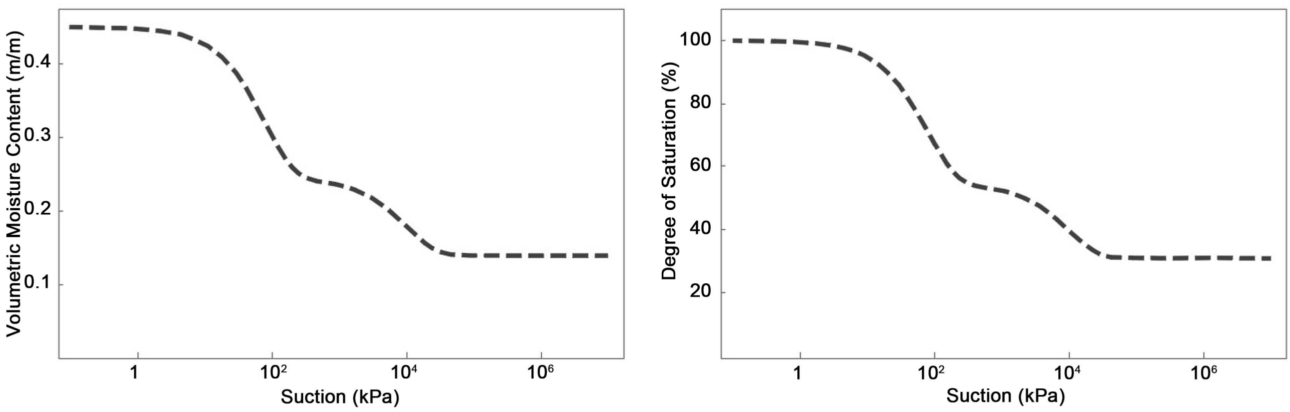

Figure 11. Soil-Water retention curve and degree of saturation for Block 4.

The determination of suction values and volumetric water content was performed through a graphical analysis, as exemplified in Figure 12.

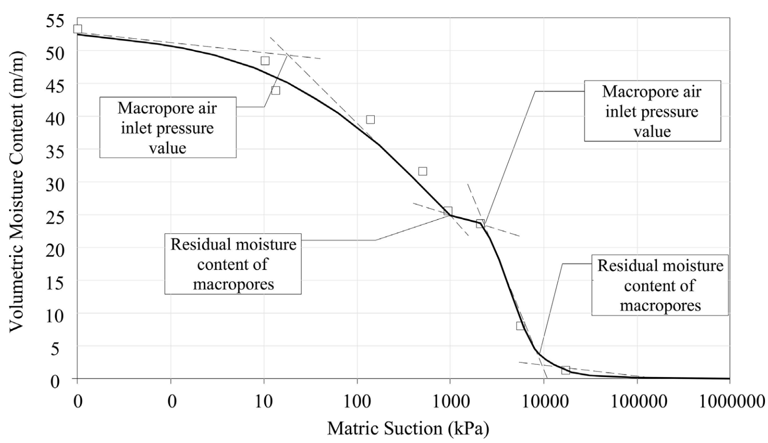

Figure 12. Parameters graph of the volumetric moisture content and suction.

This visual approach provides an intuitive and straightforward interpretation of the relationships between soil moisture and suction, facilitating a deeper understanding of the water dynamics within the soil. Additionally, this method enables the identification and characterization of the structural features of the soil's pore network, further elucidating the behavior of bimodal soils under unsaturated conditions.

5.5. Constitutive Model for Hydraulic Conductivity (K)

Building upon the formulation introduced by Cavalcante and Zornberg (2017a) in Equation (21), Costa and Cavalcante (2021a) and Costa (2022) have advanced the research by developing a specific model for the unsaturated hydraulic conductivity curve of soils with bimodal pore distribution.

This newly proposed model, presented in next equation, marks a significant milestone in the modeling of soil hydraulic properties. By incorporating the bimodal nature of the soil pore structure, the model allows for a more precise and comprehensive description of water behavior in soils exhibiting bimodal porosity characteristics.

The improved understanding provided by this model enhances its applicability to geotechnical engineering, particularly for analyzing water flow and hydraulic conductivity in unsaturated soils under varying environmental and loading conditions.

$$k(\psi) = k_s \exp(-\delta|\psi|) \tag{4}$$

$$k(\psi) = k_s \left[\lambda \exp(-\delta_1|\psi|) + (1-\lambda)\exp(-\delta_2|\psi|)\right] \tag{5}$$

The analysis of unsaturated hydraulic conductivity was conducted using data collected from Blocks 1, 3, and 4. By employing the proposed model and a computational script developed in Wolfram Mathematica®, we estimated the hydraulic conductivity curves for these specific blocks. The results, presented in **Figure 13** and **Figure 14**, demonstrate the model's effectiveness and applicability in capturing the nuances of unsaturated hydraulic conductivity. These visualizations provide a detailed perspective on the soil's hydraulic behavior under unsaturated conditions, emphasizing the influence of bimodal porosity distribution on conductivity patterns.

The results show that hydraulic conductivity within the macropores was consistently lower than that observed in the micropores, even under conditions of high suction within the micropores. For samples treated with deflocculant, the hydraulic conductivity values ranged between 10^{-4} and 10^{-6} m/s. In contrast, untreated samples without deflocculant exhibited higher conductivity, ranging between 10^{-3} and 10^{-4} m/s. These findings align with the permeability estimates obtained using Hazen's equation, based on data from the characterization tests.

The decision to estimate permeability using Hazen's formula is justified due to the low permeability values observed during the tests, which are consistent with the responses derived from the characterization data. Furthermore, the aggregate formation behavior, evidenced by the distribution of macropores and micropores in the soil-water retention curves, reinforces the relevance and applicability of this approach to the material under investigation.

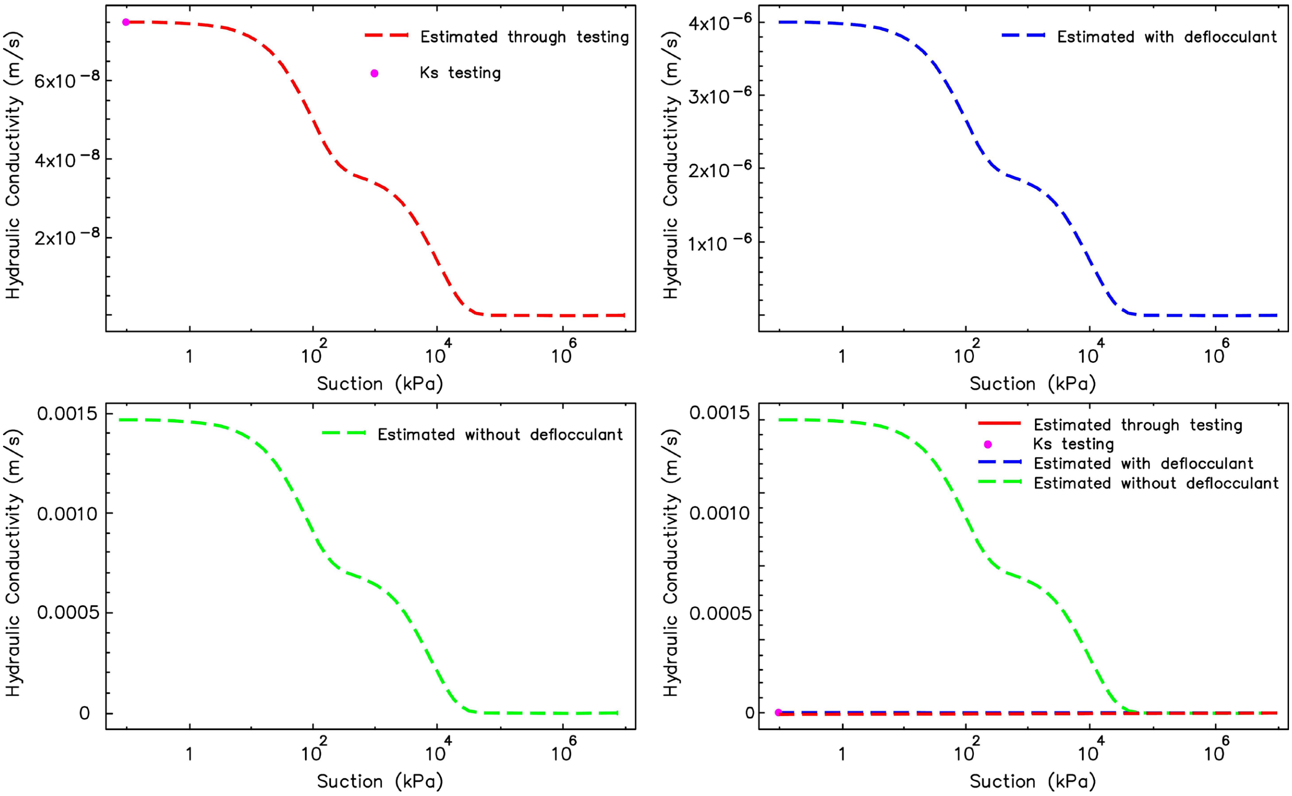

Figure 13. Bimodal hydraulic conductivity curve for Block 3, using the model proposed by Costa & Cavalcante (2021a).

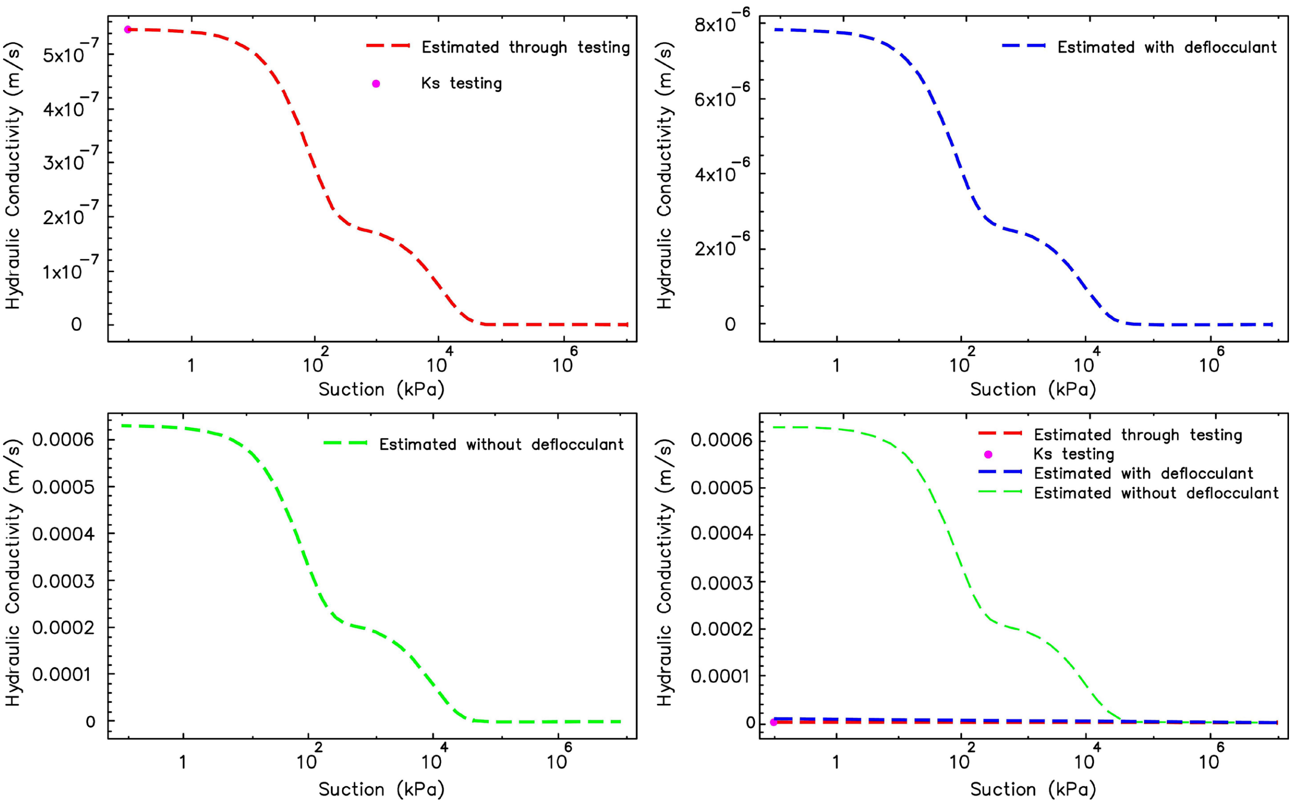

Figure 14. Bimodal hydraulic conductivity curve for Block 4, using the model proposed by Costa & Cavalcante (2021a).

5.6. Estimation of Shear Strength for Bimodal Soils

As previously presented, the phenomenon of water retention has a direct impact on the shear strength of unsaturated materials, allowing one to indirectly estimate one of these curves when the other is known.

In nature, soils may exhibit a unimodal or multimodal pore distribution, which affects the hydraulic and mechanical characteristics of these materials. In this context, this section of the study presents a shear strength model for bimodal unsaturated soils, based on the retention function proposed by Costa & Cavalcante (2021a).

To achieve this, Equation (6) proposed by Vanapalli et al. (1996) was written by Sousa (2024) considering the moisture value defined in Equation (7). Thus, the shear strength of bimodal soils can be expressed as:

$$\tau = c' + \left[(\sigma - u_a) + \left[\lambda \exp\left(-\delta_1 |u_a - u_w|\right) + (1-\lambda)\exp\left(-\delta_1 |u_a - u_w|\right)\right]^k (u_a - u_w)\right]\tan\phi' \tag{6}$$

and the effective normal stress as:

$$\sigma' = (\sigma - u_a) + \left[\lambda \exp\left(-\delta_1 |u_a - u_w|\right) + (1-\lambda)\exp\left(-\delta_1 |u_a - u_w|\right)\right]^k (u_a - u_w) \tag{7}$$

By this prerogative, it is possible to define the apparent cohesion of unsaturated soil through (Sousa, 2024):

$$c_{ap} = \left[\lambda \exp\left(-\delta_1 |u_a - u_w|\right) + (1-\lambda)\exp\left(-\delta_1 |u_a - u_w|\right)\right]^k (u_a - u_w)\tan\phi' \tag{8}$$

and total cohesion as:

$$c = c' + \left[\lambda \exp\left(-\delta_1 |u_a - u_w|\right) + (1-\lambda)\exp\left(-\delta_1 |u_a - u_w|\right)\right]^k (u_a - u_w)\tan\phi' \tag{9}$$

As shown, it is evident that the pore distribution of a material influences its mechanical and hydraulic characteristics. In this model, the resistance behavior can be separated according to the influence of macropores and micropores based on the retention and pore distribution model of Costa & Cavalcante (2021a).

Thus, for the case of κ = 1, the apparent cohesion can be easily divided into contributions from macropores (C_{ap_macro}) and micropores (C_{ap_micro}), as follows (Sousa, 2024):

$$c_{ap} = c_{ap\_macro} + c_{ap\_micro} \tag{10}$$

where:

$$c_{ap_{macro}} = \lambda \exp\left(-\delta_1 |u_a - u_w|\right)(u_a - u_w)\tan\phi' \tag{11}$$

$$c_{ap_{micro}} = (1-\lambda)\exp\left(-\delta_2 |u_a - u_w|\right)(u_a - u_w)\tan\phi' \tag{12}$$

and in this case, it is also given by:

$$\tau = c' + \left[(\sigma - u_a) + \left[\lambda \exp\left(-\delta_1 |u_a - u_w|\right) + (1-\lambda)\exp\left(-\delta_1 |u_a - u_w|\right)\right]^k (u_a - u_w)\right]\tan\phi' \tag{13}$$

or, in a more simplified notation:

$$\tau = c' + c_{ap\_macro} + c_{ap\_micro} + (\sigma - u_a)\tan\phi' \tag{14}$$

Thus, the resistance model can also be represented by the expression:

$$\tau = c' + (\sigma - u_a)\tan\phi' \tag{15}$$

and for the effective normal stress, it is obtained:

$$\sigma' = (\sigma - u_a) + \left[\lambda \exp\left(-\delta_1 |u_a - u_w|\right) + (1-\lambda)\exp\left(-\delta_1 |u_a - u_w|\right)\right]^k (u_a - u_w) \tag{16}$$

Unlike equation which describes the shear strength of unimodal soils and is easily manipulated mathematically to infer the maximum value of the function, the derivative and maximum value estimation of Equation (6) is much more complex. This is because, for κ > 1, there is a polynomial component of suction contributing to the resistance. However, when κ = 1, it is possible to deduce that the value of ψ pico for a bimodal soil is equal to:

$$\psi_{pico} = \frac{1}{\delta_2} \tag{17}$$

It is noted that for κ ≠ 1 (which generally occurs in bimodal soils), τ becomes a mixed function with respect to suction, composed of an exponential term that multiplies (ua-uw). This complicates the study of the function's domain and the mathematical definition of points of interest since the parameter κ\kappaκ is estimated solely through the fitting of shear strength test data.

For a better understanding of the shear strength model for bimodal soils proposed by Sousa (2024), a parametric analysis of Equation (6) is presented in **Figure 15**.

As shown in the parametric analysis in **Figure 15**, for the proposed bimodal shear strength model, it is observed that the contribution of smaller pores is more significant than that of larger pores to the unsaturated shear strength of bimodal soils. Thus, based on the result of Equation (17) and observing the pattern associated with the ψ_{pico} value of the unimodal model, it can be inferred that for the bimodal case with κ ≠ 1, the following relationship might hold:

$$\psi_{pico} \approx \frac{1}{\kappa\delta_2} \tag{18}$$

Thus, considering that equation applicable and valid for the proposed model in this research, the maximum shear strength of an unsaturated bimodal soil can be obtained by:

$$\tau_{pico} \approx c' + \left[(\sigma - u_a) + \frac{1}{\kappa\delta_2}\left[\lambda \exp\left(-\frac{\delta_1}{\kappa\delta_2}\right) + (1-\lambda)\exp\left(-\frac{1}{\kappa}\right)\right]\right]^{\kappa} \tan\phi' \tag{19}$$

The applicability of these last two equations will be tested in the following section using experimental shear strength data adjustments for unsaturated samples of Brazilian bimodal soils. The shear strength surface obtained through the application can be visualized in **Figure 16**.

5.7. Validation of the Constitutive Models

The validation of the constitutive models developed for the material under study was primarily based on tests conducted to determine the soil-water retention

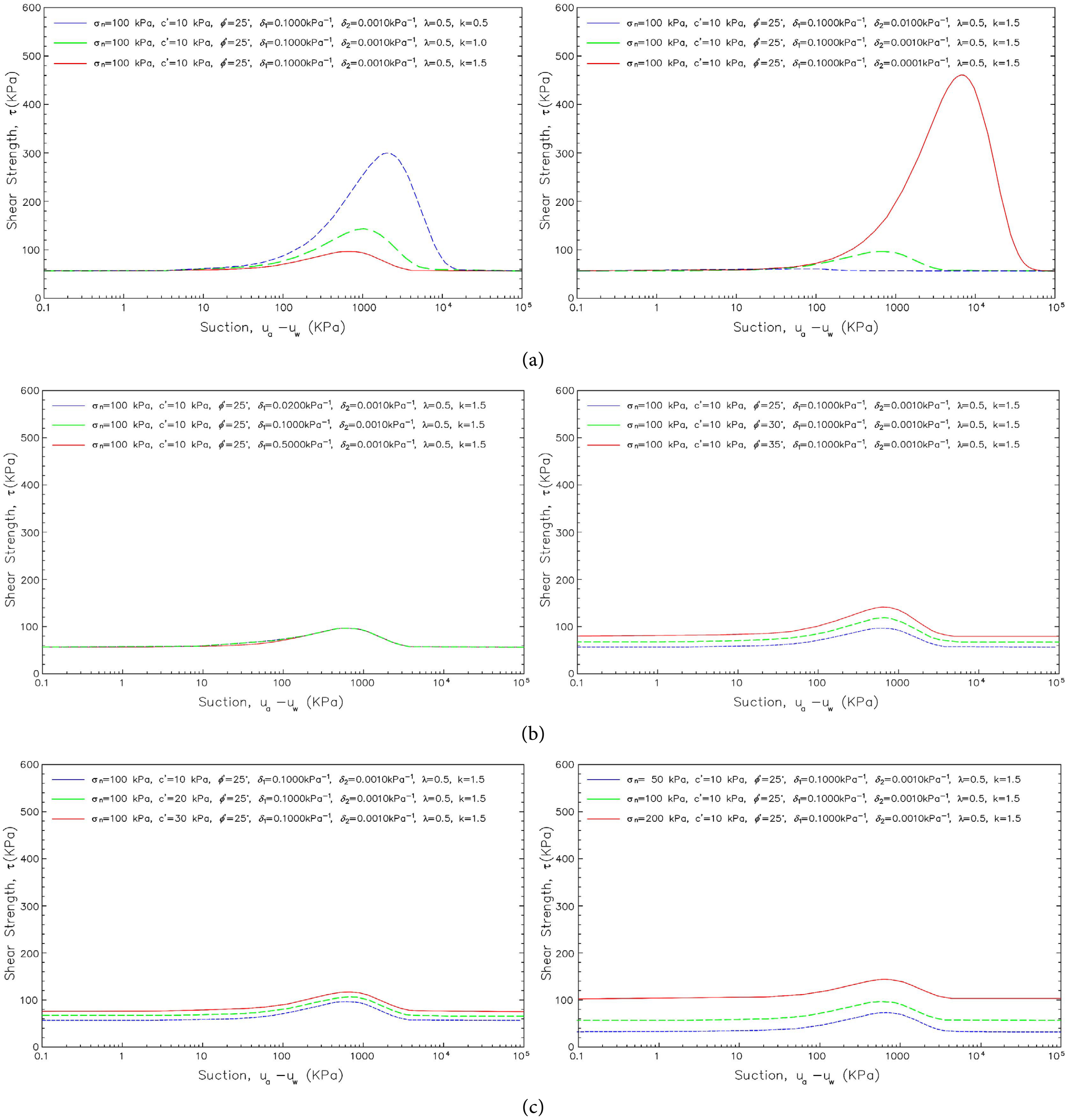

Figure 15. Parametric analysis of the bimodal shear strength model.

curve. These tests demonstrated a remarkably satisfactory alignment between the results predicted by artificial intelligence (AI), specifically using machine learning techniques, and the data obtained from laboratory experiments. A significant agreement was observed between the simulated curves and those fitted to the experimental data, as proposed by Costa and Cavalcante (2021a). This finding underscores the accuracy of the model in capturing soil behavior and reinforces the validity of the proposed constitutive models.

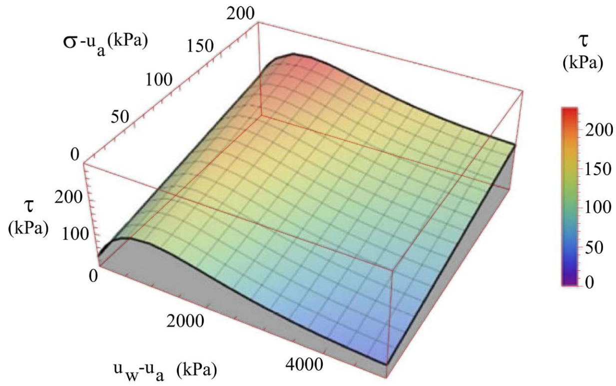

Figure 16. Example of unsaturated shear strength surface for bimodal soils (Sousa, 2024).

Moreover, the results confirm the presence of a bimodal distribution in both the soil-water retention curve and the analysis of unsaturated hydraulic conductivity. **Figure 17** and **Figure 18** illustrate the relationships between volumetric water content and the degree of saturation as a function of suction for Blocks 1 and 3, emphasizing the key findings of this study.

The initial point highlighted on the modeled curve represents the hydraulic conductivity estimated from grain size distribution test results, both with and without the addition of a deflocculant. This point is pivotal for understanding the initial influence of the soil's grain size characteristics on its unsaturated hydraulic conductivity. Moreover, it provides a key reference for interpreting the effects of deflocculant treatment in the tests.

This section focuses on the comparative analysis of unsaturated shear strength as a function of suction. The comparison involves two sets of adjustments: one obtained through advanced artificial intelligence (AI) modeling, specifically employing machine learning techniques, and the other derived from the methodology proposed by Costa and Cavalcante (2021a) (**Figure 19**).

The results are critical for assessing the accuracy and applicability of the models in predicting shear strength under unsaturated soil conditions. This analysis validates the models and highlights specific nuances, including potential advantages of one approach over the other.

Figure 20 presents the comparative results of unsaturated shear strength, demonstrating the effectiveness of adjustments obtained through AI-based modeling and the methodological approach proposed by Costa and Cavalcante (2021a). These figures highlight the capability of both methodologies to accurately capture the relationship between unsaturated shear strength and suction under varying conditions.

Figure 20 extends the comparative analysis by examining adjustments derived from AI-based modeling and those following the Costa and Cavalcante (2021a) methodology. The figure emphasizes differences in behavior between natural and saturated moisture conditions, offering deeper insights into the predictive accuracy and applicability of the respective models.

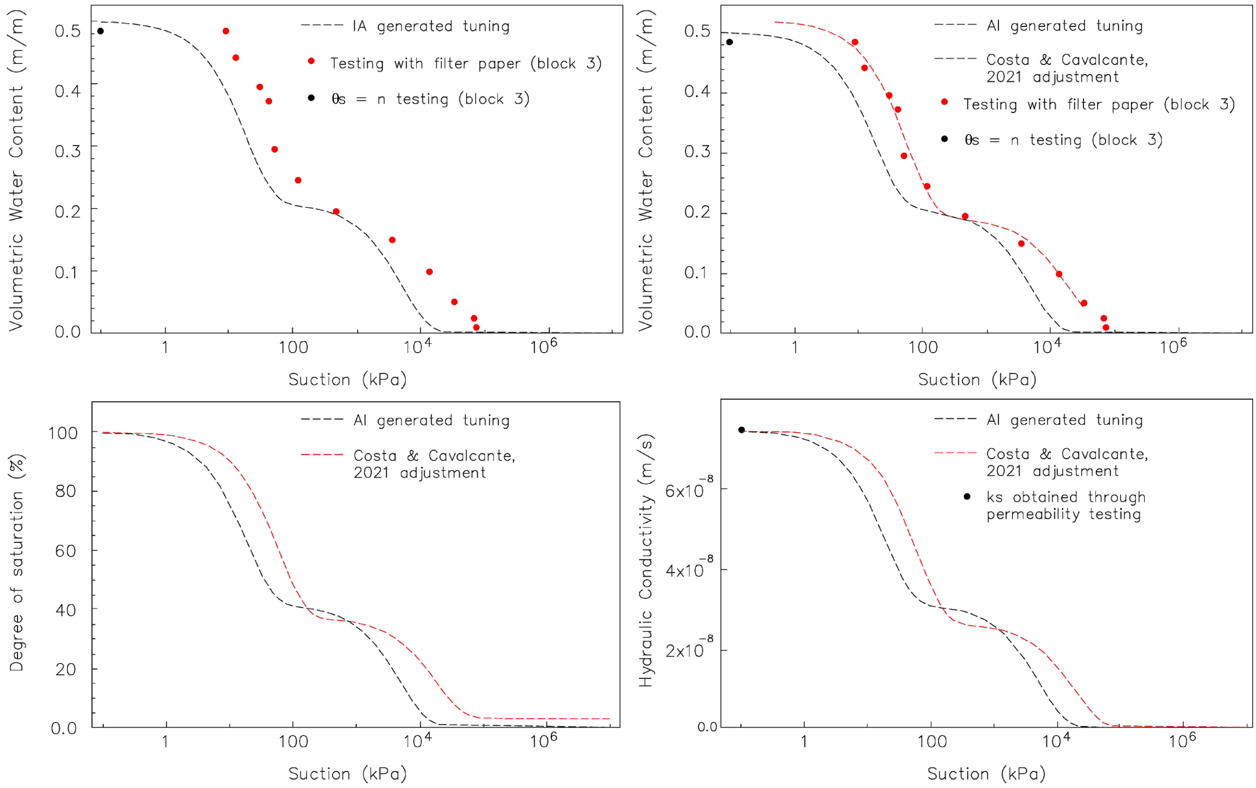

Figure 17. Variation of unsaturated hydraulic conductivity (Ks) with suction for Blocks 1 and 3.

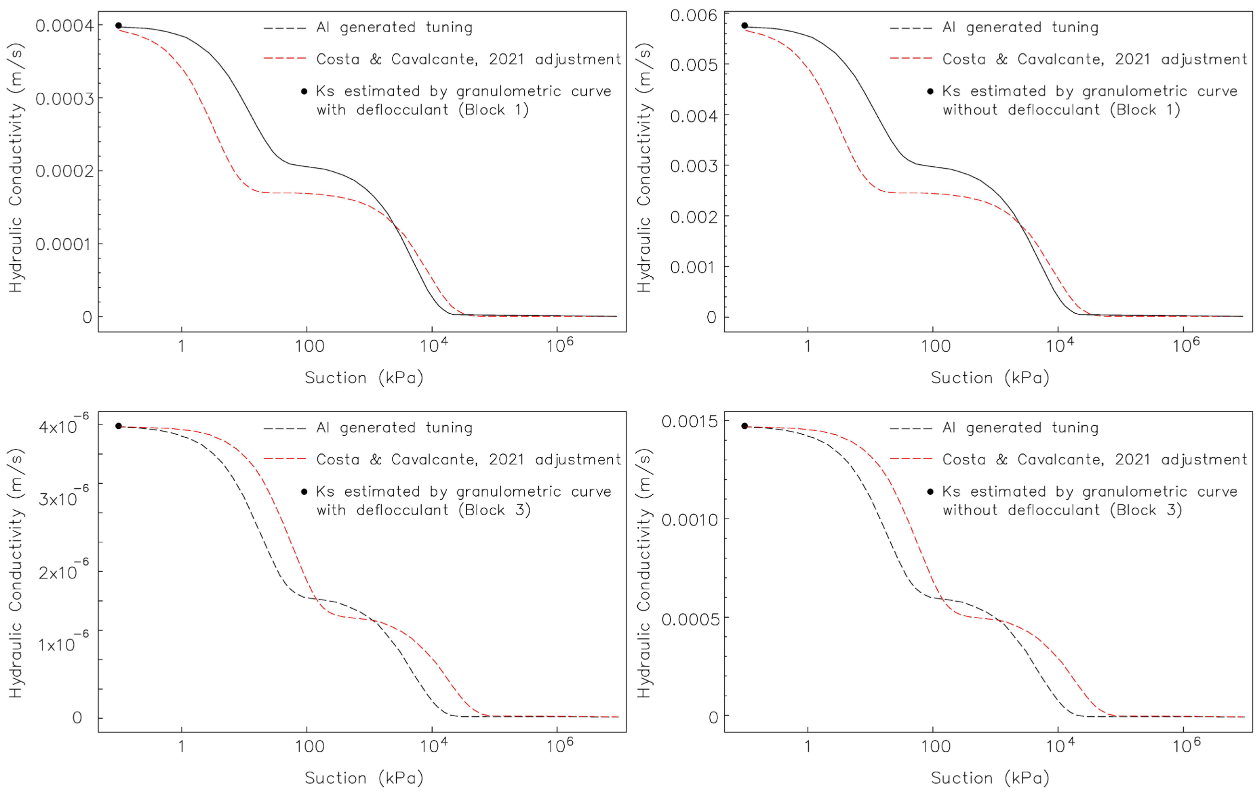

Figure 18. Relationship between unsaturated hydraulic conductivity and suction for Blocks 1 and 3. Legend: Black: Adjustments obtained through AI modeling (Machine Learning); Red: Adjustments based on the Costa and Cavalcante (2021a) model.

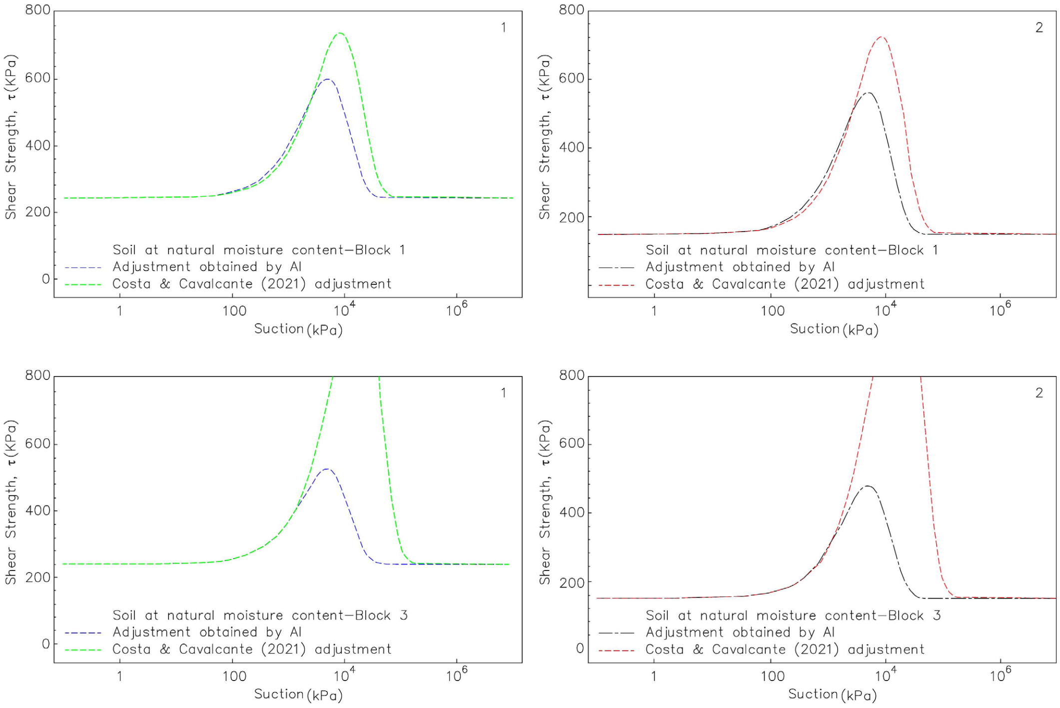

Figure 19. Relationship between unsaturated shear strength and suction variation for Blocks 1 and 3. Legend: 1) Adjustments obtained through AI (Machine Learning) modeling; 2) Adjustments based on the Costa and Cavalcante (2021a) model for natural and saturated moisture conditions.

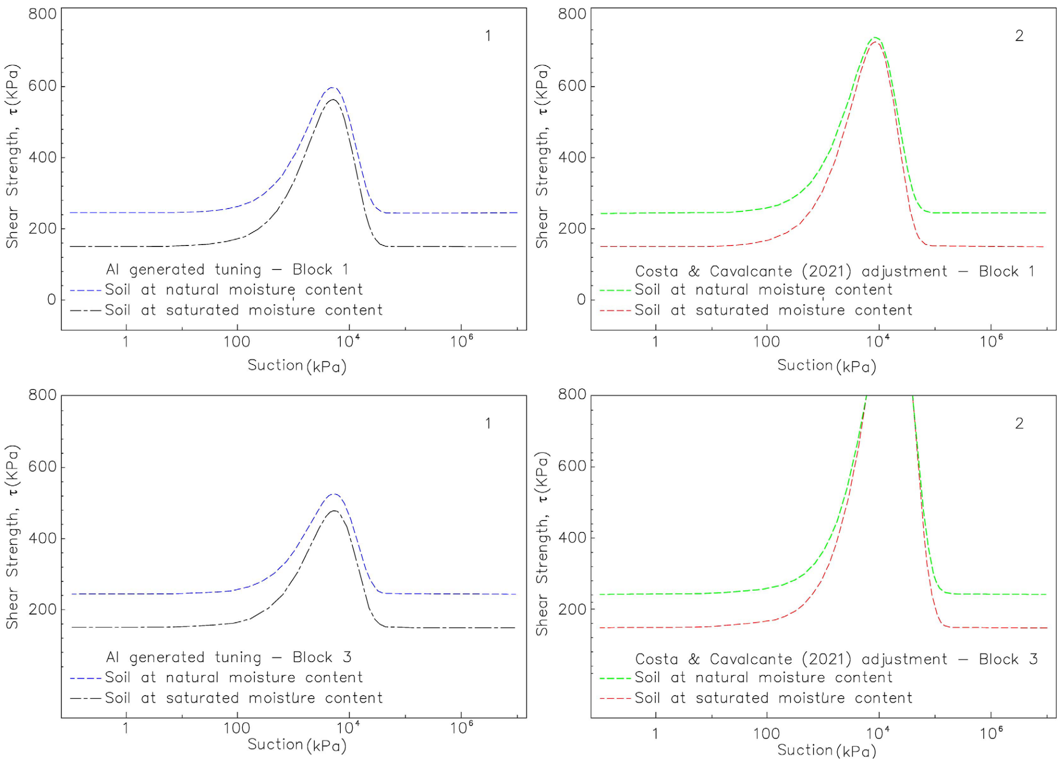

Figure 20. Relationship between unsaturated shear strength and suction variation for Blocks 1 and 3. Legend: 1) Adjustments obtained through AI (Machine Learning) modeling; 2) Adjustments based on the Costa and Cavalcante (2021a) model for natural and saturated moisture conditions.

6. Conclusion

The analyses conducted demonstrated the potential of physical and numerical modeling to understand the behavior of the materials studied. The use of artificial intelligence (AI) and machine learning (ML) techniques to determine the parameters of the soil-water retention curve, hydraulic conductivity, and shear strength under unsaturated conditions proved to be fast, effective, and suitable for the material studied, highlighting the speed and reliability in obtaining initial parameters.

Although conventional tests are important, they require time, specialized labor, and care in sample preparation. The use of machine learning emerges as a viable alternative, providing fast and reliable predictions, especially when the continuous feeding of the database with new tests increases the accuracy and reliability of the models. The more data included, the closer the models will be to real-world material conditions.

The results suggest that the studied material, despite being predominantly composed of fine particles, behaves like a granular material, forming aggregates that create macropores and micropores, typical of bimodal soils. The soil-water retention and hydraulic conductivity curves reinforce this characteristic, and the shear strength modeling exhibited behavior typical of sandy soils, with increased strength up to a peak and subsequent decline as suction increased.

The integration of the constitutive models proposed by Costa and Cavalcante (2021a), Costa (2022) and Sousa (2024) with the algorithmic code in Mathematica® software showed that the modeling processes were efficient and accurate. The use of AI, combined with laboratory tests, proved to be a powerful tool for predicting constitutive parameters, although sensitivity adjustments were necessary in some simulations due to the limitation of available data in the simulator. However, expanding the database will make future simulations more precise and reliable.

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Conflicts of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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