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An approach to aging phenomena of granular materials from UCS and DEM analysis

Una aproximación al fenómeno de envejecimiento de materiales granulares a partir de UCS y DEM

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ABSTRACT: Soil aging, a time-dependent process, manifests alterations over periods ranging from days to months, characterized by heightened small-strain stiffness and increased large-strain strength. The causative mechanisms, whether chemical or mechanical, remain uncertain, contributing to inconclusive verifications. However, studies suggest that mechanical aging predominates through increased frictional resistance and particle interlock facilitated by soil grain reorientation. This study assesses shear resistance increase in sandy materials due to mechanical aging in Ottawa and Guamo sand. Unconfined Compression Tests on cylindrical specimens (HDR 1.0), aged up to six months, reveal increases in compressive resistance of up to 15% based on particles morphometry and roughness assessed with Scanning Electron Microscopy (SEM) analysis. Furthermore, Discrete Element Analysis analyses were carried out to assess stress levels and granular morphometry and demonstrates the incidence of grain reorganization processes and interlock as aging phenomena in sands. Hence, calibration of discrete element models in PFC 2D allowed the study of granular materials based on real textural and morphometric conditions (not spherical balls), offering insights for future investigations into aging effects.

KEYWORDS: Sands aging; time-dependent changes; mechanical aging, increased interlock.

1 INTRODUCTION

The phenomenon of soil aging is a well-established concept in geotechnical engineering, defined as the time-dependent alteration in the behavior of sandy soils (Bowman & Soga, 2003). This alteration, which becomes significant over periods ranging from days to months, is often characterized by an increase in small strain stiffness and increases in shear strength (Baxter & Mitchell, 2004; Daramola, 1980; Tatsuoka et al., 2000, 2002). Despite its significance, the underlying causes, and mechanisms of soil aging, particularly in granular materials, remain a subject of ongoing investigation and discussion within the scientific community (Toyota & Takada, 2021). This lack of clarity presents challenges in inconclusive verifications (Wang et al., 2008).

Numerous studies have contributed to our understanding of soil aging, and they suggest that it can be attributed to either mechanical or chemical mechanisms (Baxter & Mitchell, 2004; Bowman & Soga, 2003; Mesri et al., 1990; Mitchell, 2008; Nakarai & Yoshida, 2015). Nevertheless, it's worth highlighting that there have been relatively fewer studies on time-related phenomena in sand compared to the extensive research conducted on clay, as pointed out by Augustesen et al. (2004). Based on the above, the mechanical mechanism underlying soil aging can be explained as an increase in frictional resistance or enhanced interlocking of particles resulting from the reorientation of soil grains, leading to the compaction of granular materials (Zaitsev et al., 2014). Furthermore, mechanical aging in soils can be linked to geological origin and historical stress conditions, both of which contribute to rheological changes in the bonding forces between soil particles (Castilla-Barbosa et al., 2023; Troncoso & Garcés, 2000).

Several authors demonstrated that the mechanical mechanism for aging is interpreted, in general terms, as an increment in frictional resistance or increased interlock of particles developed by reorientation of soil grains and rearrangements, causing compaction of granular materials due to particle movements and rotations that lead to re-distribution of the stress in soil skeleton. Furthermore, they found that this phenomenon is intricately linked to a range of main geotechnical properties, such as small strain stiffness, cone penetration resistance, liquefaction resistance (related to Cyclic Stress Ratio - CSR), and shear strength, among other characteristics of these materials' behavior (Afifi & Woods, 1971; Bowman & Soga, 2003; Bwambale & Andrus, 2019; Joshi et al., 1995; Leung et al., 1996; Ltifi et al., 2014; Murphy, 1982; Nasiri et al., 2022; Omunguye et al., 2018; Suarez et al., 2014; Thomann & Hryciw, 1992; Towhata et al., 2015, 2017; Wang et al., 2008; Wang & Tsui, 2008; Wang, 2017; Wright & Hornbach, 2021; Zaitsev et al., 2014).

Furthermore, as highlighted by Sachan (2008) and Yan et al. (2009), the geometric arrangement of particles, referred to as micro fabric, exerts a significant influence on shear strength properties, such as the friction angle. Therefore, a precise characterization of the soil surface is crucial for comprehending the forces at play between soil particles (Gómora-Herrera et al., 2018). It's worth noting that surface roughness generates bonds between particles, while microfabric reflects the imprints of geological history, stress conditions, depositional environment, and weathering history within the soil deposit. Consequently, a comprehensive analysis of microfabrics at various scales is indispensable for discerning their impact on interparticle forces and the phenomenon of soil aging.

2 MATERIALS AND METHODS

To comprehensively understand the role of micro-fabric in particle interlocking and the progression of mechanical aging within fine sands, particularly in the transition zone with silts, a multifaceted investigation has been proposed. This endeavor integrates experimental methodologies with advanced numerical analyses. By employing a combination of techniques, ranging from microscopic examination to computational modeling, this approach aims to elucidate the intricate interactions between particle micro-structure and mechanical behavior, shedding light on the complex dynamics governing sediment mechanics in these granular materials.

In the first instance, an experimental stage was implemented to ensure an accurate description of the particles surface and morphometry which is essential to understanding forces between soil at the microscale in fine sands and the transition range with cohesionless silts. On the other hand, a numerical analysis through Discrete Element Methods models is proposed from the use of Particle Flow Code - PFC (Itasca) under a two-dimensional condition that preserves the properties of unconfined compression tests (specimen dimensions and deformation conditions), considering the micro-fabric of the particles and their incidence in the mechanical performance. Furthermore, the proposed model will consider the superficial micro-texture and morphometry of sand particles under study, based on the analysis of electronic microscopy images (SEM), to preserve the angularity and textural properties.

To assess the impact of mechanical processes on the onset of aging phenomena in fine sand, it became imperative to characterize the superficial properties of geomaterials employed in this study. Experimental tests were conducted on two distinct sands: Ottawa Sand and Guamo Sand (Figure 1). Both sands under analysis showed a fine distribution based on the Udden--Wentworth grain-size scale, from sieve No. 16 (1.18 mm) to sieve No. 200 (75 µm).

2.1 U*nconfined Compression Tests (UCS)*

The uniaxial compressive strength (UCS) test is another widely used calibration test in DEM simulations as presented by Gao-Feng (2015). Moreover, UCS is commonly associated as a measurement in control and comparison purposes of improved soils and may be usefully to calibrate constitutive models as reported Spagnoli et al. (2021). UCS samples were fabricate with 5\% of water content to the dry mass with height-diameter ratio of 1.0 (sample diameter 50 ± 2 mm) and were tested with a fixed deformation-controlled rate of 1.50 %/min on a INSTROM 3300 Series Universal Testing Systems. Furthermore, sand samples were compacted to a 75% of Relative Density for UCS tests.

2.2 *Semi-assisted techniques to Image analysis*

Quantitative measurements of grain size, roundness, and angularity (as factors that could affect the interlock phenomena) were analyzed with a Scanning Electron Microscopy (SEM). SEM image analysis is a highly energetic and focused electron beam, and imaging is carried out by using the emission of secondary electrons for topography interpretation, and back-scattered electrons for atomic number lecture (Girão et al., 2017). However, it is relevant to highlight that in the case of non-conductive samples, such as sands, it was necessary to cover the surface of the sample with a very thin layer of gold to make it conductive and allow the interaction with the electrons.

As part of the identification of sands under analysis, Scanning Electron Microscopy (SEM) observations were executed to identify the morphometry and textural surface as key facts that could affect particle interaction and interlock phenomena. SEM Analysis were carried out with a Zeiss EVO HD15 Scanning Electron Microscope apparatus under electron high tension (EHT) voltage up to 20 kV, with a thin gold cover over the sand particles and high-vacuum condition. Moreover, SEM analysis was carried out with a working distance from 5 mm up to 9.5 mm, an energy range of 20.0 (keV), and an output rate from 8.000 to 12.000 cps., and a high vacuum condition. Moreover, the image analysis of the confined compression tests, with a view to determining failure patterns and displacements, is carried out from the implementation of the Zeiss GOM Correlate Pro tool based on the image correlation algorithm and point tacking. The images from UCS were shoot with a Sony Alpha A7III 4K Mirrorless at intervals every 2 second from the beginning of the test until the failure of the specimen.

Figure 1. Fine-medium Ottawa (upper) and Guamo (below) sands particles under study, based on the Unified Facilities Criteria (U.S. Army Corps of Engineers, 2022).

2.3 Discrete Element Method (DEM) simulation analysis

The Discrete Element Method (DEM) was conceived by Cundall and Strack in the early 1970s as a computational technique tailored for simulating the behavior of granular materials. Since its inception, DEM has found applications in diverse fields, including geotechnical engineering, physics, and materials science. Consequently, investigating aging- or creep-related phenomena in sand has become a focal point of research, with DEM serving as a powerful tool for simulating sand changes in bulk behavior (Coetzee & Scheffler, 2023), and exploring the underlying mechanisms. However, it's essential to acknowledge that there remain several unresolved challenges in the modeling process (Zhang & Wang, 2016).

On the other hand, Particle Flow Codes (PFC), developed by Itasca Consulting Group for DEM simulations of the behavior of granular mediums based on individual particles, have played a significant role in most sand aging studies. In the PFC model, particles interact at contacts between them using a generalized internal force, calculating interactions in dynamic time steps to attain states of equilibrium (Li et al., 2017). Contact mechanics are modeled through particle-interaction laws, employing a soft-contact approach where all deformations occur at the contact points between rigid bodies (Figure 2). These particle-interaction laws are commonly referred to as contact models, and their considerations have gained relevance within aging modeling studies.

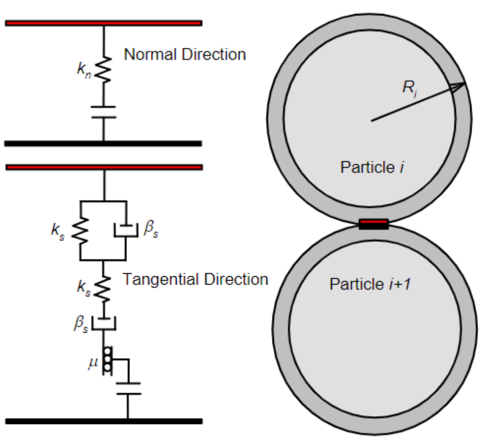

Figure 2. Behavior and rheological components of the Hertz contact model implemented in PFC from Itasca Group.

Several authors conducted investigations into various aspects of aging and mechanical behavior in granular materials, particularly sands. Wang et al. (2008) utilized DEM simulations to study aging induced by contact creep, observing a redistribution of contact forces leading to enhanced stiffness and strength in aged samples. Kuhn & Bagi (2009) explored the impact of particle incidence on assembly characteristics, noting a decrease in peak compressive strength with assembly size. Kwok & Bolton (2010) revisited frictional interactions in sands, highlighting the role of low velocity sliding in creating a strong microstructure. Likewise, Yimsiri & Soga (2010) investigated aging effects under different shearing conditions, finding that shear direction influences stiffness, strength, and dilatancy.

However, most DEM models simulated particles as Spheres to evaluate the incidence of liquefaction resistances, stiffness increase, and shear strain increases in granular materials based on the Hertz-Mindlin contact model. In fact, the Hertz-Mindlin model stands out as a prominent and versatile tool. Rooted in the classical Hertzian contact theory and enriched by the Mindlin frictional interactions between particles, this computational framework offers a nonlinear formulation based on an approximation of the theory of Mindlin & Deresiewicz (1953). With its ability to capture complex interactions between particles, the Hertz-Mindlin model serves as a potent means to simulate and comprehend the intricate dynamics of aging sand.

Based on the above, Hertz–Mindlin theory was adopted, with Normal (k_n) and Tangential contact stiffness (k_s) estimated as a function of the shear modulus (G), Poisson's ratio (υ), equivalent particle radius $\tilde{R}$, and the overlapping between particles U_n. Hence, summarized properties are presented in Table 1.

$$k_n = \frac{G\sqrt{2\,\tilde{R}\,U_n}}{1-\upsilon} \qquad (1)$$

$$k_s/k_n = \frac{2\,(1-\upsilon)}{2-\upsilon} \qquad (2)$$

Table 1. DEM Parameters adopted for Aging analysis.

Parameter	*Guamo Sand*	*Ottawa Sand*
Density of solids (kg/m^3)	2650	2700
Particle Shear modulus (GPa)	29	29
Initial Void Ratio	0.15	0.12
Poisson's ratio	0.3	0.3
Inter-particle friction coefficient	0.5	0.5
Number of Particles	3913	3900

3 RESULTS AND DISCUSSION

In the first instance, it is unrealistic to idealize granular materials with angular nature as spherical (3D) or ball (2D) models, as the angularity and roundness significantly impact particle interlock and, consequently, mechanical aging processes. To address this, the morphometry of study sand particles was identified through analysis of Electron Microscopy images (SEM)- This allowed for estimating the geometry to preserve its angularity properties (Figure 3 and Figure 4).

The fine sands under investigation (Ottawa and Guamo Sand) manifest distinct characteristics. Initially, Ottawa particles are characterized by greater roundness, their textures softened by the deposition of silica on their surfaces, impacting both textural aspects and surface roughness (Figure 3). Conversely, Guamo sand particles display a highly angular nature, marked by pronounced points resulting from fracturing during the extraction process. This aspect significantly influences particle interlock and their accommodation in response to changes in shear stress conditions.

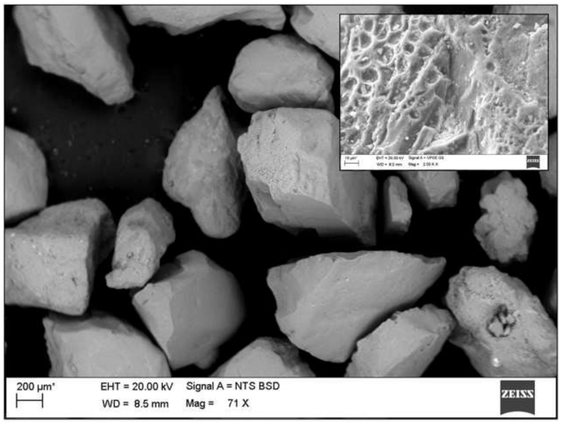

Figure 3. Scanning Electron Microscopy (SEM) images from Guamo Sand.

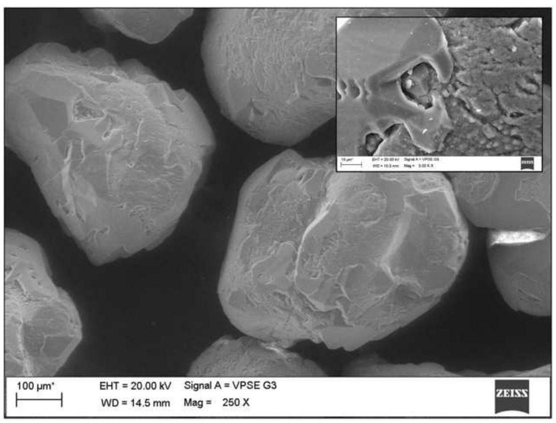

Figure 4. Scanning Electron Microscopy (SEM) images from Ottawa Sand.

The SEM identification process entails selecting the most characteristic form of each sand type under investigation, aiming to accurately capture its structure and morphological features. Every modeled particle is finely tuned to the data obtained from these observations, ensuring a precise representation of the morphological diversity present in the original sample. This approach allows for a more accurate interpretation of deformation phenomena and mechanical behavior in the studied material by effectively aligning the morphological properties of the modeled particles with real-world observations.

Regarding the contact model, the calibration extends to each contact zone between adjacent particles, ensuring an accurate representation of interactions at the microscopic scale. This calibration process considers not only the shape and morphology of the particles but also their mechanical properties and the nature of the surrounding materials. Each interaction between particles, across each of the more than 3900 generated particles, has been refined to accurately reflect experimental conditions and observed behavior in the real material (Figure 6). This attention to detail in calibrating the contact model allows for a more precise simulation of deformation and failure phenomena in the material, capturing even the subtleties of interactions at the microscopic level.

The analysis of images from UCS tests reveals a notable escalation in primary deformations during the initial compression stages of sand specimens. These deformations stem from the rearrangement of grains, with observed magnitudes extending up to 0.7%. It is noteworthy to emphasize that this phenomenon aligns closely with the predictions of the micromechanical model (Figure 6). This model aptly replicates both the presence of micro-shear bands formed within the central region of the specimen and the external conditions influenced by initial corner collapses. Moreover, increasing the axial load induces greater deformation conditions in both the radial and upper zones, serving as the initial propagation point (Figure 5). Deformations observed in sand specimens propagate from the radial to the middle zones, reaching magnitudes of up to 8.5% before failure. It's worth noting that the generated failure planes exhibit angles ranging between 59.90 and 61.10° (Figure 7 and Figure 8). Based on the Mohr-Coulomb failure criterion under a radial stress condition of 0.0 kPa, it's possible to estimate apparent cohesion conditions of up to 0.70 kPa in the sands under examination.

Similarly, the procedures for determining deformation analysis were deduced from the sequence of grain movement under the applied axial load. These observations were conducted via image analysis using the "ZEISS INSPECT Correlate" system. Consequently, unconfined compression tests facilitate the assessment and characterization of the failure mechanisms exhibited by the materials under investigation, the identification of predominant failure patterns crucial for the Discrete Element Micromechanics (DEM) model, and the prediction of maximum deformations reaching up to 13.5% prior to the sand structure's collapse.

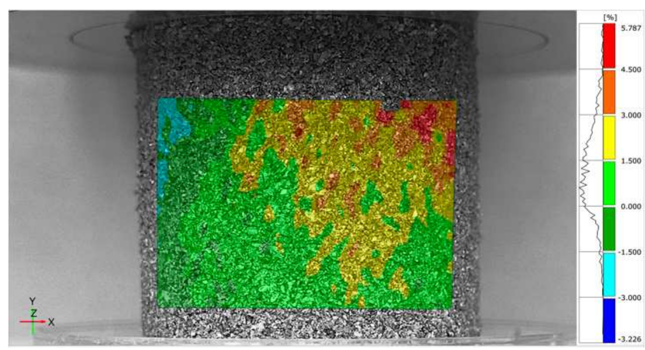

Figure 5. Scanning Electron Microscopy (SEM) images from Ottawa Sand.

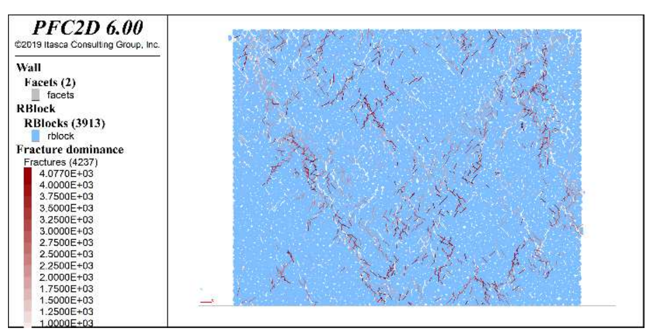

Figure 6. DEM model calibration through UCS failure pattern (5.5% deformation).

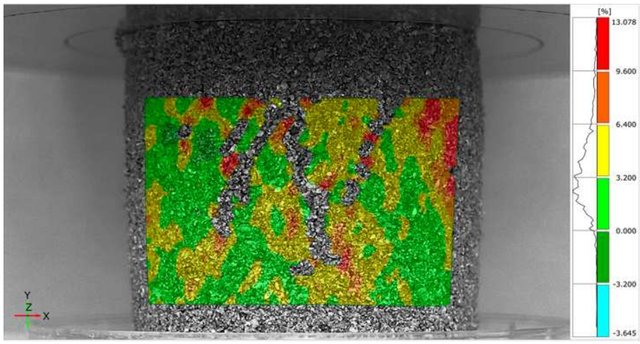

Figure 7. Unconfined Compressive Test failure pattern (13% deformation).

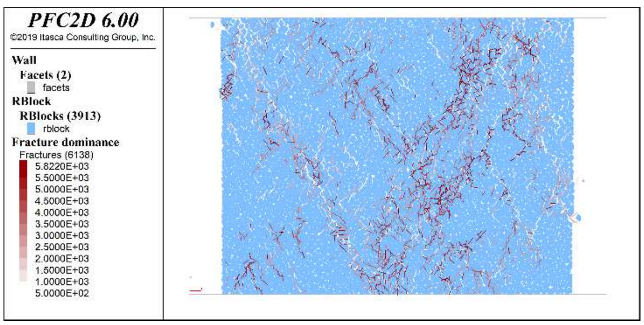

Figure 8. DEM model calibration through UCS failure pattern (13% deformation).

As aforementioned, the failure observed in the UCS test revealed fault angles of up to 62°, a characteristic that has been corroborated with the fractures observed in the micromechanical model. This validation is based on the Rosette presented in Figure 9, where most fractures exhibit inclinations of either 60° or 120° (indicating that the crack maintains its inclination but changes its direction). This alignment between experimental observations and model predictions underscores the fidelity of the micromechanical approach in capturing the intricate failure mechanisms exhibited by the material under compression.

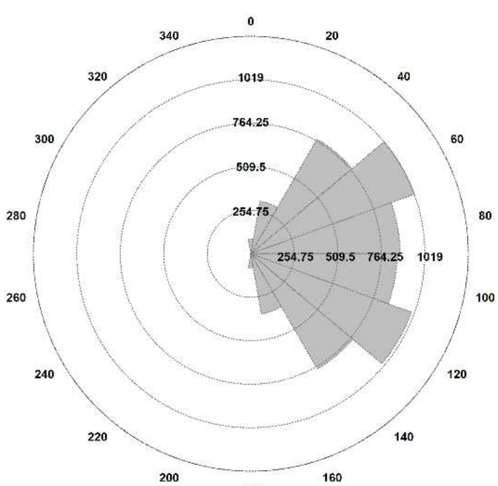

Figure 9. Rosette Analysis of Fracture Inclinations in DEM Unconfined Compressive Test.

An aging analysis conducted on fine Guamo and Ottawa sands has revealed notable enhancements in uniaxial compressive strength over periods of up to 6 months. Specifically, Ottawa sands exhibited an increase of up to 7.1%, while Guamo sands demonstrated a remarkable boost of up to 14.08%. This observed trend underscores the influence of morphometry and surface roughness, particularly in sands with a higher degree of angularity, such as Guamo sands. Moreover, the maximum strength values for Ottawa sands in their initial condition were recorded at 7.85 kPa, while aged conditions showed values of up to 9.29 kPa. In contrast, for Guamo sands, unaltered conditions (as evidenced by triplicate analyses) reached maximum values of 12.05 kPa, increasing to up to 13.33 kPa under aged conditions (Figure 10).

The analysis reveals intriguing insights into the behavior of these sands under low stresses, up to 10 kPa, in axial conditions within the specimens under study. Notably, the sands with higher angularity (Guamo) exhibit distinctive responses, suggesting a nuanced interplay between angularity, stress levels, and morphometric characteristics. Additionally, micro-mechanical modulations through Discrete Element Method (DEM) simulations have been employed to assess the behavior of sands under normal and aged conditions. These modulations have showcased significant adaptations, exhibiting variations of up to 5% compared to the stress-strain curves obtained from real Uniaxial Compressive Strength (UCS) tests. This supplementary approach offers a more detailed insight into the underlying mechanisms influencing the sand's strength, enabling a better understanding of its behavior under various conditions and its evolution over time.

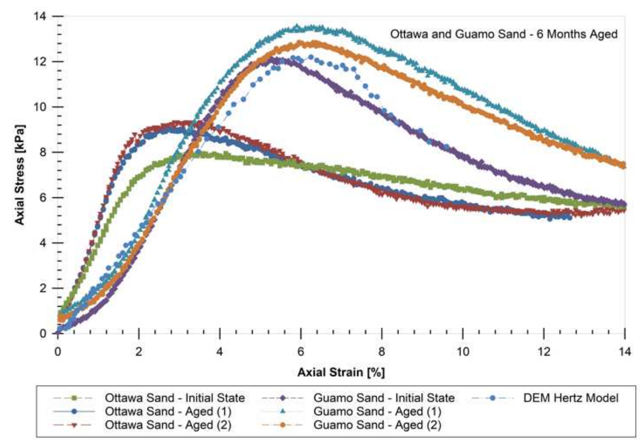

Figure 10. UCS Stress-Strain analysis on aged fine sands samples.

2 CONCLUSIONS

Soil aging presents a multifaceted phenomenon characterized by significant alterations in mechanical properties over varying timeframes, from short-term to long-term durations. While these changes typically manifest as heightened stiffness and strength, the underlying mechanisms driving soil aging remain elusive. This lack of clarity poses challenges in achieving conclusive verifications, as evidenced by divergent theories regarding the dominant factors—whether chemical processes involving cementation forces or mechanical processes driven by frictional resistance and particle interlock.

The findings of this study provide valuable insights into the role of mechanical aging in augmenting shear resistance, particularly in two commonly studied sands, Ottawa and Guamo sands. Through comprehensive testing and analysis, including Unconfined Compression Tests and Discrete Element Analysis, significant increases in compressive resistance were observed in specimens aged over a six-month period. Furthermore, the calibration of discrete element models in PFC 2D enabled the examination of granular materials under real-world textural and morphometric conditions, offering a more accurate representation of aging effects.

Likewise, the study highlights the significant influence of particle morphometry on the mechanical properties of sandy materials, as demonstrated by the comparison between Ottawa sand and Guamo sand. Ottawa sand, with its rounded particles and smoother surface, exhibits comparatively smaller changes in compressive resistance than Guamo sand, characterized by angular particles and greater surface roughness. These findings underscore the importance of considering particle shape and surface characteristics in understanding the aging behavior of granular materials. The observed increases in compressive resistance, particularly pronounced in Guamo sand, emphasize the role of mechanical aging in enhancing shear resistance over time.

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