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A continuum-discrete hierarchical multi-scale computational framework for modelling mechanical behaviors of MICP-treated soil: Part I Micro-scale investigation

Yupeng Jiang, Tirtho Sarathi Saha
IBNM, Leibniz Universität Hannover, Germany

ABSTRACT: Microbially Induced Calcite Precipitation (MICP) offers a sustainable and cost-effective approach to soil improvement by enhancing stiffness and strength through microbial-induced cementation. Despite its potential, current computational models fall short in accurately simulating the elastoplastic behavior of MICP-treated soils, particularly in representing microstructural phenomena such as bond degradation and contact anisotropy. These limitations hinder broader field-scale applications and the reliability of predictions. To address these gaps, we propose a hierarchical multi-scale modeling framework that seamlessly integrates micro-scale particle interactions, calcite morphology, and macro-scale soil behavior. This innovative approach will enable accurate simulation of elastoplastic responses post-MICP treatment, advancing both the understanding and practical application of MICP. By overcoming existing computational challenges, this framework aims to establish a robust foundation for optimizing MICP as a next-generation soil improvement technique. In this research, we initiate an investigation into the influence of interparticle bonding by employing a state-of-the-art numerical framework. This approach couples the material point method (MPM), utilized to model calcite bonds, with the discrete element method (DEM), which represents the individual soil grains. The results of our study provide new insights into the de-bonding mechanisms of soils treated with microbial-induced calcite precipitation (MICP), thereby establishing a foundation for improved predictions of their mechanical behavior.

KEYWORDS: MICP-treated soil, calcite precipitation failure, continuum damage mechanics, MP-DEM coupling method.

1 INTRODUCTION

Microbially Induced Calcite Precipitation (MICP) represents a significant advancement in soil improvement methodologies, distinguished by its favorable environmental profile, affordability, and minimal carbon emissions. The technique leverages the metabolic functions of microorganisms to foster calcite precipitation, thereby creating cohesive bonds between soil grains. This process serves to augment the soil's collective stiffness and load-bearing capacity while generally maintaining its permeability. The increasing prevalence of both academic studies and practical deployments worldwide highlights the promise of MICP as a next-generation technology for ground engineering.

MICP is primarily driven by microbial ureolysis, where bacteria hydrolyze urea to increase soil alkalinity, causing calcium carbonate to precipitate and bridge soil particles. This process requires adequate pore space for bacterial transport and a continuous supply of calcium and urea. Once formed, calcite bonds are chemically stable under typical geotechnical conditions, though they remain susceptible to dissolution in highly acidic environments or mechanical failure if stresses exceed the bond strength.

A fundamental prerequisite for assessing the efficacy of MICP and quantifying the resulting soil stiffness is a clear understanding of the mechanical response of the inter-grain cementation. Experimental investigations have systematically sought to clarify the relationship between calcite deposition and the observable patterns of failure. Among these, the comprehensive study by Ham et al. (2022) is particularly noteworthy. By subjecting cemented bead pairs to tensile and shear loading, they identified three distinct failure classifications based on their locus relative to the grains—interfacial debonding, internal fracture, and a mixed mode—and confirmed that these modes significantly dictate the ultimate strength of the cementation.

Despite these experimental contributions, the fundamental mechanisms that determine the operative failure mode remain largely unresolved. This ambiguity contributes to the variable and often suboptimal outcomes observed in MICP applications. There has been no systematic elucidation of the key parameters—such as calcite volume and interfacial topography—that control the failure response across a range of loading scenarios. Consequently, it is imperative to conduct focused investigations using computational tools, as they provide the necessary means to probe the micro-scale mechanics that govern these complex failure processes.

In this study, we aim to develop a micro-mechanical model of a calcite-cemented grain pair, which will serve as the Representative Volume Element (RVE) in a future multi-scale simulation framework. To accurately capture brittle failure within this RVE, we adopt the framework of continuum damage mechanics, enabling a rigorous simulation of cementation degradation under both tensile and shear loading. To effectively model grain-calcite interactions, we employ the material point-discrete element method (MP-DEM). Specifically, the calcite and its damage evolution are represented using the material point method (MPM), while its bonding with the grains—simulated as discrete elements—is coupled through the MP-DEM framework. Our results for this RVE indicate that failure modes are collectively governed by calcite content, cementation topography, and the in-situ forces acting on the grain pair.

2 MICRO-SCALE SIMULATION FOR INTER-PARTICLE BONDS

2.1 Small strain theory with stress objectivity

We adopt the small-strain theory, considering the high stiffness of calcite and the relatively minor strain that develops before cementation failure. Meanwhile, to account for the varying displacements of grain boundaries, we employ the Jaumann stress rate to ensure the objectivity of stress state measurements, which can be expressed as:

$$\dot{\sigma}_{ij} = \dot{\sigma}_{ij}^{J} + \sigma_{ik}\Omega_{jk} + \sigma_{jk}\Omega_{ik}, \quad (1)$$

where $\dot{\sigma}_{ij}^{J}$ denotes the Jaumann stress rate and Ω_{jk} is the spin rate. The use of objective stress rate can be express by the stiffness matrix $\boldsymbol{C}$ with strain rate $\dot{\boldsymbol{\varepsilon}}$ as:

$$\dot{\boldsymbol{\sigma}}^{J} = \boldsymbol{C} : \dot{\boldsymbol{\varepsilon}}. \quad (2)$$

to eliminate the influence of the rotation.

2.2 *Constitutive models*

To fully capture the material anisotropy of bio-precipitated calcite, we in-corporate experimental data from existing studies. These studies suggest that a vertically transverse isotropic (VTI) model (Best et al.,2024) is more appropriate for rep-resenting its constitutive behavior, considering its lower stiffness due to its bio-origin and lack of consolidation.

2.3 *Continuum Damage model*

In consistence with the material anisotropy, we adopt the second-order damage tensor for the evolution of damage state inside the calcite cementation which can be written as:

$$\boldsymbol{\sigma}_e = \mathbb{M}:\boldsymbol{\sigma}, \tag{3}$$

where $\mathbb{M}$ is a fourth-order tensor that constructed by the identity tensor $\boldsymbol{I}$ and damage tensor $\boldsymbol{D}$ with:

$$\mathbb{M} = \frac{1}{4}\left(\boldsymbol{\phi} \underline{\otimes} \boldsymbol{I} + \boldsymbol{\phi} \overline{\otimes} \boldsymbol{I} + \boldsymbol{I} \underline{\otimes} \boldsymbol{\phi} + \boldsymbol{I} \overline{\otimes} \boldsymbol{\phi}\right), \tag{4}$$

$$\boldsymbol{\phi} = (\boldsymbol{I} - \boldsymbol{D})^{-1}. \tag{5}$$

The surface of the damage potential is further expressed as:

$$F^D(\boldsymbol{Y}, B_0) = Y_{eq} - B_0 = 0, \quad Y_{eq} = (\frac{1}{2}\boldsymbol{Y}:\boldsymbol{Y})^{\frac{1}{2}}, \tag{6}$$

where B_0 is the material constant for the damage surface, and $\boldsymbol{Y}$ and the thermal dynamic force of damage development that can be derived with the Helmholtz free energy ψ as:

$$\boldsymbol{Y} = -\rho\frac{\partial\psi}{\partial\boldsymbol{D}}. \tag{7}$$

2.4 *Coupling between grains and calcites*

In this work, we leverage the material-point discrete element method (MP-DEM), a powerful hybrid numerical scheme ideal for simulating cemented granular materials (Jiang et al., 2020 & 2022). The method's strength lies in its dual representation: the calcite cementation, which undergoes complex deformation and damage, is modeled as a continuum using the material point method (MPM), while the soil grains, which remain rigid, are efficiently represented as discrete elements (DEM). This approach not only enhances computational efficiency by simplifying the grain representation but also adeptly handles the moving boundaries of the cement as the grains displace.

The core of the MP-DEM framework is the numerical algorithm that couples the continuum material points with the discrete elements. This interaction is managed through a penalty-based projection method. The fundamental goal is to enforce kinematic constraints at the grain-cement interface, ensuring that the material points representing the calcite adhere to the surface of the discrete elements representing the grains.

This coupling is realized through the calculation of a specific force, the coupling force $\boldsymbol{f}^p_{cpl}$, which acts on the material points at the interface as:

$$\boldsymbol{f}^p_{cpl} = \mathcal{F}(\boldsymbol{q}_0, \boldsymbol{q}_t), \tag{8}$$

where $\boldsymbol{q}_0$ and $\boldsymbol{q}_t$ denotes the initial and current vector between a material point and the center of mass of corresponding grains it attached to.

Its calculation begins by projecting the state of the discrete element onto the material points to determine a "target" position for each point. If a material point's calculated position after a time step does not coincide with this target position (i.e., a relative displacement or "penetration" occurs), the penalty-based projection function, $\mathcal{F}$, is invoked. This function calculates a restoring force that is proportional to the magnitude of this kinematic incompatibility. This force, $\boldsymbol{f}^p_{cpl}$, effectively "pulls" the material point back towards the grain surface, enforcing the bond. Simultaneously, this process ensures the action-reaction principle is satisfied by applying an equal and opposite force to the discrete element. This crucial step guarantees that the mechanical response of the deforming calcite, including the build-up of stress and initiation of damage, is faithfully transmitted to the grains, governing their subsequent motion and the overall system dynamics.

With this method, the material points representing the calcite cementation are categorized into two groups: those directly attached to the grain surfaces (attached) and those that are not (unattached), as shown in Figure .1. Cementation in these two groups exhibits distinct damage patterns, ultimately leading to different failure modes.

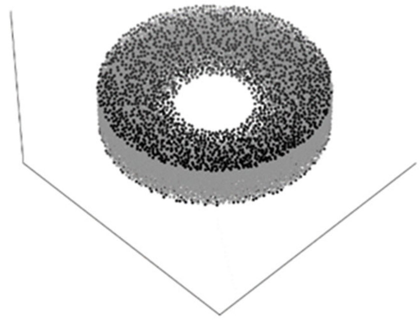


Figure 1. The attached and unattached material points denoted by dark and light color respectively

3 SIMULATION SETUP

In this study, we numerically investigate the failure patterns of three distinct cementation configurations under tensile loading, which were previously examined by Ham et al. (2022) and are illustrated in Figure 2. The configurations are categorized based on calcite content and morphology: ‘coating,’ in Figure 2. (a) where a low percentage by weight of calcite coats the grain surfaces; ‘meniscus’ in Figure 2. (b) where a medium to high calcite content forms a meniscus-shaped bridge between the grains; and ‘flat’ in Figure 2. (c) where a high calcite content results in a cylindrical bond. Following the precedent set by Ham et al. (2022), our analysis identifies three primary failure modes: ‘debonding mode,’ characterized by the detachment of calcite from the grains; ‘internal mode,’ where failure occurs within the calcite bond itself due to tensile loading; and ‘mixed mode,’ which involves a combination of the two aforementioned mechanisms.

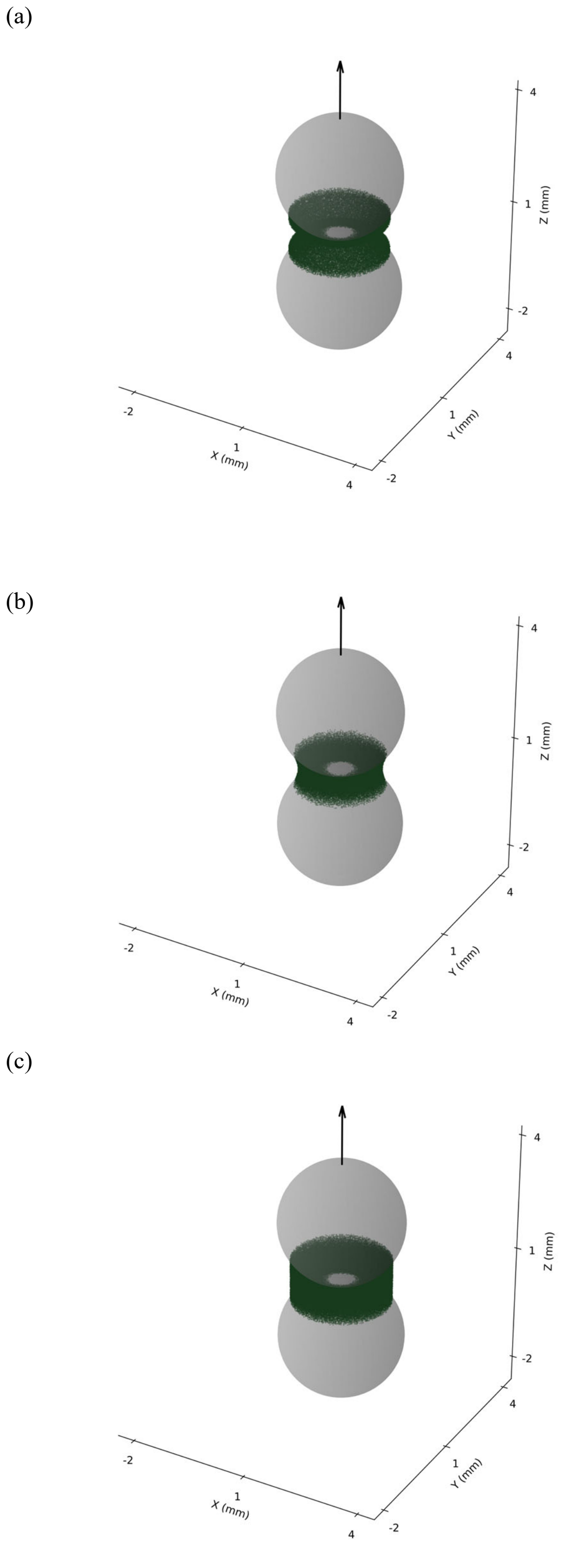


Figure 2. The simulation setup. (a) coating cemetation,(b) miniscus cementation, and (c) flat cemetation.

4 SIMULATION PARAMETERS

In this simulation, the selection of model parameters is guided by the principle of parsimony, with the overarching goal of developing a computationally tractable multi-scale framework. By intentionally minimizing the number of free parameters, we aim to create a model that is not only efficient but also less susceptible to overfitting, thereby enhancing its generalizability and reducing the need for extensive calibration at the macro-scale.

This objective is made possible by our choice to explicitly resolve the calcite bond using a continuum-based method. Unlike discrete element models that often represent cementation through simplified, abstract contact laws, our approach allows for the direct implementation of physically meaningful material properties. The parameters governing the calcite's behavior—namely its elastic moduli, tensile strength, and damage evolution characteristics—are standard solid mechanics properties. As such, their values can be directly informed by or measured from targeted laboratory experiments on bulk calcite, as demonstrated in recent studies (e.g., Best et al., 2024). This direct link to experimental data ensures that our micro-scale model is physically grounded, a critical feature for building a reliable bottom-up multi-scale simulation.

We only present the parameters that were required for calibration in Table.1; the rest of physical parameters can be retrieve from the references

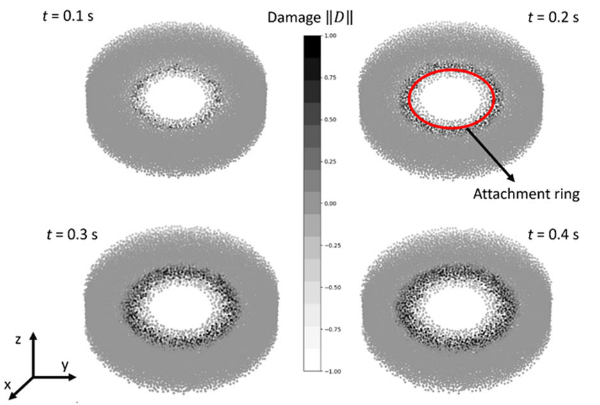
Table 1. Simulation parameters required for calibration

Parameter	Symbol	Value	Unit
DEM radius	r	5	mm
Contact normal coefficient	k_n	9.6	GPa
Contact shear coefficient	k_t	0.96	GPa
Time step size	dt	1e-9	s
Damage surface	B_0	9.6e-3	GPa
Damage cut-off	D_{cut}	0.9	-

5 RESULTS AND ANALYSE

The initial results from our tensile loading simulation, employing the flat torus-filling model for calcite cementation, reveal a distinct failure mechanism governed by its unique geometry. In this configuration, the calcite adheres to the grain surfaces not at a single point, but across a continuous, ring-shaped region. This toroidal contact geometry is critical, as it facilitates a more uniform distribution of strain along the entire grain-cement interface. Consequently, the bond exhibits high resistance to interfacial debonding, as localized stress peaks that would typically initiate peeling or detachment are effectively minimized.

Instead of interfacial failure, the simulation shows that damage initiation and localization occur within the calcite material itself, specifically in the region immediately adjacent to the attachment ring. This phenomenon is attributed to a significant stress concentration that develops at the geometric discontinuity where the main body of the calcite cement meets the toroidal attachment zone. As tensile load increases, micro-cracks initiate in this high-stress region and subsequently propagate in a coplanar, ring-like manner, effectively "cutting" the bond away from its anchor point. Therefore, the observed failure pattern is a direct consequence of the interplay between a strong, well-distributed bond interface and the inevitable stress concentration arising from the cementation's geometry under tensile loading. This internal fracture mode demonstrates that for certain cementation topographies, the cohesive strength of the calcite, rather than the adhesive strength of the interface, becomes the limiting factor in the system's performance.



Figrue 3. The evolution of the internal damage in the calcite with flat configuration

Simultaneously, the evolution of interfacial bond damage under tensile loading was monitored, revealing a distinct debonding mechanism. The damage was observed to propagate in a concentric, ring-shaped manner, a phenomenon attributable to the axisymmetric stress state induced by the spherical grain geometry at the bonding interface.

Interestingly, the progression of this damage was not continuous but occurred in discrete stages, creating a pattern analogous to tree rings. This discrete behavior is directly influenced by the implemented damage threshold (D = 0.9), as the failure of one complete ring of bonds precedes the initiation of damage in the next. Moreover, the rate of damage accumulation was found to be asymmetric across the ring's width. The inner perimeter of the damage ring consistently grew faster than the outer perimeter. This is a direct consequence of stress concentration: the smaller radius of the inner circumference results in a higher localized stress, which in turn accelerates the degradation of the bond.

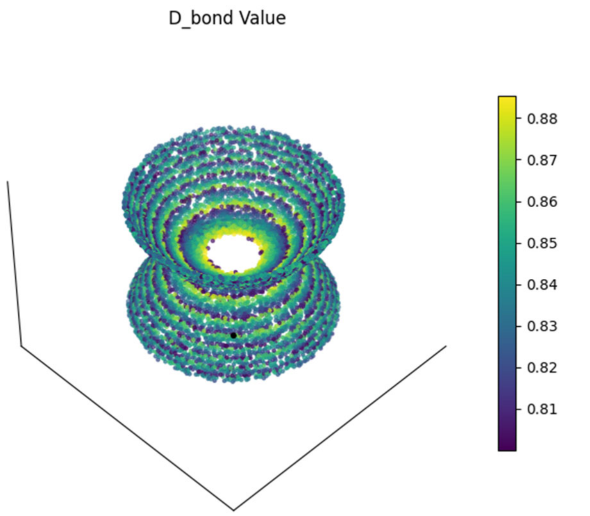


Figure 4. The evolution of the damage and debonding for coating configuration.

6 CONCLUSIONS

In conclusion, our simulations demonstrate that the failure mechanism of calcite cementation is critically governed by its geometric topography. The flat torus model, with its continuous ring-shaped contact, distributes stress effectively to resist interfacial debonding. Consequently, failure is dominated by an internal cohesive fracture, driven by stress concentration at a geometric discontinuity. When interfacial debonding does occur, it exhibits its own distinct signature: a discrete, concentric "tree-ring" propagation, also governed by stress concentration. These findings reveal a clear competition between cohesive and internal failure, where the cementation geometry ultimately dictates which mode prevails and determines the bond's strength.

This study focuses on coarse-grained soils that allow free bacterial transport. The findings have limited applicability to fine-grained or clay soils, where narrow pore throats restrict bacterial migration, leading to localized clogging rather than uniform cementation. Furthermore, the electrochemical and cohesive forces dominant in clays differ significantly from the contact-based mechanics modeled here, necessitating alternative constitutive approaches for those soil types.

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