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MACRO- AND MICRO-BEHAVIORS OF SOIL WITH SOLUBLE PARTICLES DURING 1D COMPRESSIONAL TESTS USING 3D DEM SIMULATION

Truong Q. Hung[1], Khoa M. Tran[2], Ngoc Quy Hoang[3*]

Abstract – *Micro- and macro-behaviors of soils are significantly affected by soluble particles such as salts. To investigate the macro- and micro-behaviors of soil specimens with soluble particles, this study adopted the discrete element method to model a conventional one-dimensional compression test (oedometer) for a sample of 10% salt. Salt particles are created to be softer compared to sand particles. The 3D discrete element method model was validated by laboratory experimental results carried out in a previous study. The oedometer was conducted by applying loads from 5 kPa to 640 kPa. Macro- and micro-behaviors of the specimen were investigated by observing several parameters, including vertical strain, porosity, vertical and horizontal stress, and contact force during compression. The simulation results showed that the 3D discrete element method model approximately relocated laboratory experimental results, with a high correlation to vertical strain and void ratio. The lateral earth pressure ratio continuously decreased during loading. Moreover, observation of the force chain during loading revealed a rearrangement of soil particles and enhancement of inter-particle contacts. The macro- and micro-behaviors of soil with soluble particles could be effectively investigated using the 3D discrete element method model. The model provided a reliable framework for capturing the macro- and micro-mechanical properties of granular mixtures with soluble grains under confined compression. However, the dissolution of the sample was not implemented. Future research could focus on the dissolution phenomenon in the 3D discrete element method model to provide a deeper understanding of soluble particles on soil behaviors, particularly under changing environmental conditions.*

Keywords: DEM, granular, microstructure, oedometer, soluble.

I. INTRODUCTION

The mechanical behavior of granular materials containing soluble particles is highly sensitive to their initial fabric, which governs critical properties such as shear resistance, deformation patterns, and stiffness. Previous studies revealed that even when granular assemblies have identical bulk densities, differences in particle arrangement and contact orientation can lead to significant variations in shear strength [1, 2]. In particular, distinct initial fabric conditions result in different responses under triaxial compression and extension, highlighting the influence of microstructural anisotropy on mechanical performance.

Soluble soils are often encountered in the foundations or abutments of dams and other earth structures [3, 4]. When these soluble constituents dissolve due to changes in groundwater chemistry or environmental conditions, the internal fabric of the soil matrix is disrupted. This dissolution can degrade the soil's mechanical integrity, potentially leading to settlement or even catastrophic structural failure, as observed in several historical cases [3]. As soluble particles are removed, the soil becomes looser, less stiff, more compressible, and exhibits reduced strength compared to its original state [4, 5]. The reduction in passive

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[1] Van Lang School of Technology, Van Lang University, Vietnam

[2,3] Department of Civil and Environmental Engineering, University of Waterloo, Canada

*Corresponding author: nqhoang@uwaterloo.ca

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earth pressure caused by particle dissolution may elevate the slope instability, while the loss of solid parts of the soil will weaken the bearing capacity of the foundation [6, 7]. These changes highlight the importance of understanding both the macro- and micro-scale consequences of particle dissolution in granular soils.

Despite increasing awareness of these issues, current research on the behavior of granular soils containing soluble particles remains limited, particularly in terms of capturing the macro and micro responses during mechanical loading. Therefore, this study aims to fill this gap by employing the discrete element method (DEM) to simulate one-dimensional compressional behavior-specifically, the oedometer test on soil mixtures that include a fraction of soluble particles. By integrating particle-scale observations with stress–strain behaviors, a link is established between microstructural evolution and engineering-scale performance. Ultimately, the findings are expected to contribute to more reliable predictions of soil behavior in geotechnical applications where dissolution processes are critical.

II. LITERATURE REVIEW

The oedometer test is a widely used and standardized method in geotechnical engineering that provides essential information on soil compressibility, settlement behavior, and stress-strain characteristics, which are crucial for the design and analysis of foundations and earth structures [8, 9]. While the mechanical response of granular soils under confined one-dimensional loading has been widely examined, few studies have addressed the effects of dissolution on granular soils under at-rest earth pressure (K_o loading conditions), largely due to the complexities involved in implementation [10, 11]. This has limited the understanding of how granular soils with evolving internal structures, such as those with dissolving particles, behave under more realistic in-situ stress paths.

The DEM, originally introduced by Cundall et al. [12], has proven to be a powerful numerical tool for modeling the behavior of granular materials at particle and system levels [1, 2]. DEM facilitates the analysis of particle-scale interactions and enables the development and calibration of constitutive models that link micro-mechanics to macro-scale behavior. In this method, the soil medium is modeled as an assembly of discrete, rigid particles within a computational domain. Particle interactions are described using a soft-contact approach, and the system evolves through the application of Newton's laws of motion and force-displacement relationships at each time step [12].

In Vietnam, DEM studies have been widely applied to investigate the micro- and macro-mechanical behaviors of granular soils. For example, the DEM simulation of the shear behavior of granular soils shows that the bonding width plays a crucial role in enhancing shear strength and strongly influences mechanical characteristics such as the dilatancy angle and particle rotation [13]. Another investigation for two-dimensional DEM proposed a four-step procedure for preparing granular samples and a minimum number of particles for ensuring sample quality under isotropic compression [14].

The objective of this study is to investigate the macro- and micro-scale behaviors of granular mixtures containing soluble particles during one-dimensional compression using 3D DEM simulations. In the model, a specimen is constructed by randomly generating sand particles mixed with 10% soluble particles by volume. Compression is applied by translating the top and bottom boundaries, simulating vertical loading under confined conditions. Both macro- and micro-level responses are evaluated throughout the compression process. Parameters such as vertical strain, porosity evolution, contact forces, and internal stress distributions are analyzed to provide insight into the effects of particle dissolution on the mechanical response of the soil.

III. MODELING OF GRANULAR SOILS USING DEM

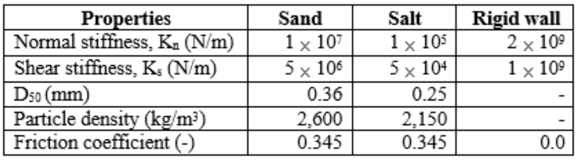
A. *Material properties*

To simulate oedometer tests, a three-dimensional DEM model was developed using particle flow code (PFC), a widely used DEM software by Itasca [15]. In the study by Truong et al. [4], laboratory experiments were conducted to investigate the small-strain stiffness characteristics of sand–salt mixtures with varying salt contents (0–10% by volume). The specimens, prepared with a constant initial void ratio, were tested in a brass oedometer cell equipped with bender elements to measure one-dimensional compressibility and shear wave velocity simultaneously. The testing program consisted of different salt contents with different vertical stresses applied at the time of dissolution. Dissolution was induced by saturating the samples with a dilute NaCl solution, and changes in vertical strain, void ratio, and shear wave velocity were monitored during loading, unloading, and reloading stages. Therefore, in the model, the granular soil mixture was represented by spherical particles mimicking sand and soluble particles (e.g., salt), while rigid planar boundaries simulated the confinement of an oedometer cell. The model setup was designed to replicate the laboratory conditions with particle properties closely aligned with those used in the physical experiments, as summarized in Table 1 [4].

Sand particles were assigned a mass density of 2,600 kg/m^3 and a normal contact stiffness of 107 N/m, values typical for quartz-rich mineral grains. The sand particles were uniformly distributed with a median diameter (D_{50}) of 0.36 mm. Soluble particles, representing salt, were modeled as smaller spherical particles with D_{50} = 0.25 mm and a significantly lower normal stiffness of 10^5 N/m, reflecting the softer nature of salt crystals compared to quartz. Both sand and salt particles were assigned to the same inter-particle friction coefficient of 0.345 to simulate consistent shear interaction at contacts.

To replicate one-dimensional compression and prevent lateral deformation, the oedometer cell was modeled with rigid lateral, top, and bottom walls. These walls were assigned a stiffness 100 times greater than that of the sand particles and were modeled with zero friction to minimize wall resistance and allow for controlled vertical compression.

Table 1: Input parameters



Properties	Sand	Salt	Rigid wall
Normal stiffness, K_n (N/m)	1×10^7	1×10^5	2×10^9
Shear stiffness, K_s (N/m)	5×10^6	5×10^4	1×10^9
D_{50} (mm)	0.36	0.25	-
Particle density (kg/m^3)	2,600	2,150	-
Friction coefficient (-)	0.345	0.345	0.0

B. Sample generation

The DEM specimen was constructed with a cylindrical shape measuring 74 mm in diameter and 63 mm in height. The granular assembly contains a total of 62,104 sand particles and 12,918 salt particles, corresponding to a 10% volume fraction of soluble particles, as shown in Figure 1. Figure 1 illustrates the DEM representation of the soil specimen, highlighting the spatial distribution of sand and salt particles within the confined domain.

It is important to note that the salt particles are smaller in size than the sand particles, with a D_{50} of 0.25 mm compared to 0.36 mm for sand. The design of particle size and selection allows salt particles to occupy void spaces between larger sand grains, influencing the overall microstructure and mechanical behavior of the specimen during compression [4].

The initial packing process is meticulously designed to establish a baseline sediment structure. It begins with the random placement of designed particles within a higher volume of the designed cylinder domain under conditions of zero gravity and zero inter-particle friction. The initial height of the samples is created at a level of 20% higher than the target sample. This frictionless and weightless state allows the particles to be freely positioned without premature settling or clustering. Subsequently, the sample of designed particles is created by moving the upper cap of the cylinder cell to the designed height and void ratio of approximately 63 mm and 0.76, respectively, which corresponds to a relatively dense granular assembly typical of natural sediments before alteration. The sample, at the final stage of generation, has a diameter of 74 mm, a height of 63 mm, and a void ratio of 0.76, and consists of two types of particles: sand particles with a D_{50} of 36 mm and soluble particles with a D_{50} of 25 mm. Two rigid caps, upper and lower caps, were vertically moved to compress the sample to the designed pressures, and the rigid cylinder wall was used to simulate the confined condition of the sample during loading.

Once this target porosity is reached, interparticle friction is activated with a coefficient of 0.345, reflecting moderate frictional resistance akin to that observed in many sandy soils. Simultaneously, gravitational forces are introduced to simulate realistic weight effects.

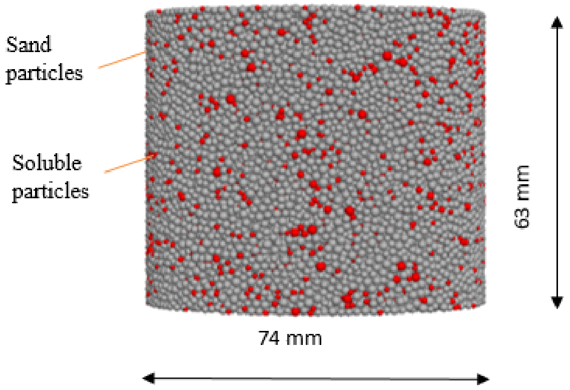


Fig. 1: 3D DEM specimen in PFC

Note: grey particles represent sand grains; red particles represent soluble grains

C. One-dimensional confined loading

A series of conventional oedometer tests was simulated in this study to investigate the compressional behavior of granular soils containing soluble particles. The loading sequence was designed to replicate typical laboratory procedures, with successive loading steps applied at effective stress levels of 5, 10, 20, 40, 80, 160, 320, and 640 kPa while maintaining constrained lateral strain. The constrained lateral strain condition mimics a confined (earth pressure at rest), commonly encountered in subsurface soil layers, ensuring that the sediment's response is constrained laterally as it would be in a natural or engineered setting.

Vertical compression was applied through a wall servo-control mechanism, which allows for precise manipulation of the translational motion of the top and bottom walls. The servo function adjusts wall velocity dynamically to apply or maintain a specified vertical force, thereby achieving the desired loading condition. In this simulation setup, the target load was prescribed in terms of force rather than stress, with the force applied over the wall area corresponding to the desired effective stress levels.

D. Measurement sphere

To monitor key mechanical responses during compression, a measurement sphere with a radius of 20 mm was placed at the center of the specimen, as illustrated in Figure 2. This measurement region allows continuous, real-time tracking of parameters, such as porosity, stress, and strain, throughout the loading process. Data from the measurement sphere were recorded at every mechanical time step, providing a detailed history of local changes in the specimen's internal state. Due to its central location and size, the parameter readings obtained from the sphere are considered representative of the overall behavior of the soil specimen under one-dimensional compression.

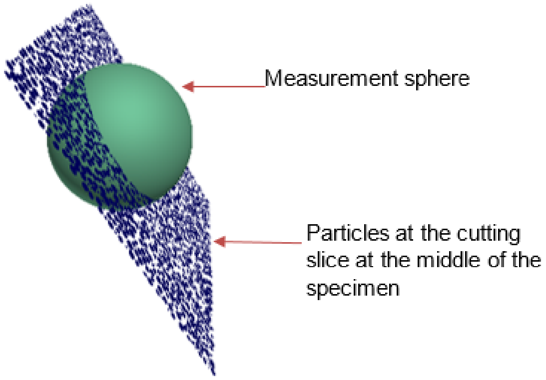


Fig. 2: Measurement sphere

IV. RESULTS AND DISCUSSION

A. Vertical strain

The numerical simulation results are summarized and presented in Figure 3, alongside the laboratory experimental data for comparison. Figure 3 illustrates the variation in vertical strain, calculated as the ratio of the specimen's settlement to its initial height, throughout the loading process under constrained lateral strain (K_o-loading) conditions. The DEM simulation closely reproduces the experimental trends, especially at the final loading stage (640 kPa), where both methods yield a comparable vertical strain of approximately 0.024%.

However, during the intermediate loading stages, particularly between 40 kPa and 320 kPa, the simulation exhibits slightly lower strain values than those observed in the experiments. This discrepancy may be attributed to reduced wall friction effects in the numerical model. In the simulation, the lateral, top, and bottom boundaries were designed with minimal or no friction to better isolate vertical compression.

Despite these minor differences, the DEM model successfully captures the overall deformation response of the specimen, suggesting that it is a reliable tool for investigating the macro-mechanical behavior of granular mixtures containing soluble particles.

B. Void ratio

The void ratio was calculated from the DEM simulation and plotted against the vertically effective stress in Figure 4. The numerical results were compared with the corresponding results from laboratory oedometer tests. Similar to the vertical strain trends, Figure 4 demonstrates a strong correlation between the DEM simulation and experimental data during both the initial (low stress) and final (high stress) loading stages. However, a noticeable discrepancy is observed during the intermediate loading steps, particularly at 160 kPa and 320 kPa, where the DEM results slightly deviate from the laboratory measurements. These variations may be attributed to the friction between particles and rigid walls. Besides matching the experimental results, the compression curve from the numerical simulation of the oedometer test in the mixture of particle assemblies containing soluble grains also exhibits good agreement with the one-dimensional confined compression response reported in McDowell et al. [10]. The results indicated that the stress levels considered in the two studies are not identical.

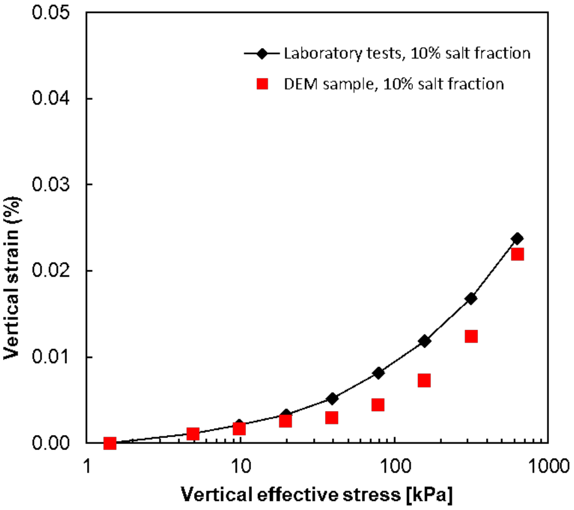


Fig. 3: Vertical strain versus vertical effective stress

C. Lateral earth pressure ratio

Lateral earth pressure ratio, K_o, is evaluated based on the ratio of horizontal effective pressure and vertical effective pressure under the condition of confined one-dimensional loading. Obtaining real-time K_o during laboratory experiments is complex due to the complication of measuring real-time horizontal stress. Therefore, K_o is usually estimated from internal friction angles, which is not real-time. A high friction angle indicates a low K_o and vice versa. However, for the DEM model, observing K_o is much more convenient using the measurement sphere. K_o is calculated using vertical and horizontal stresses measured during compression and plotted in Figure 5. At light compression steps (5 and 10 kPa), K_o expresses very high values, approximately

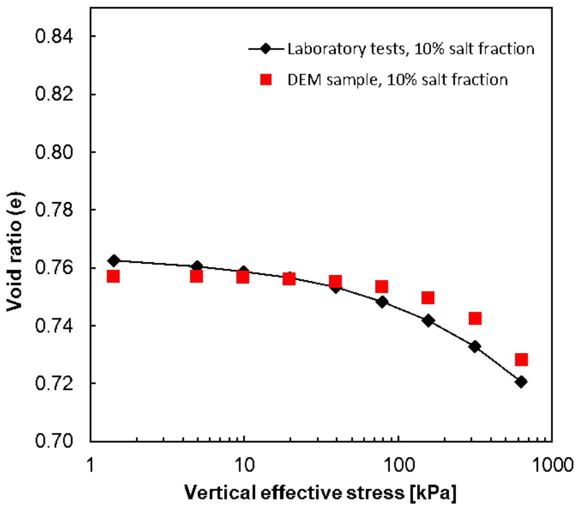


Fig. 4: Void ratio versus vertical effective stress

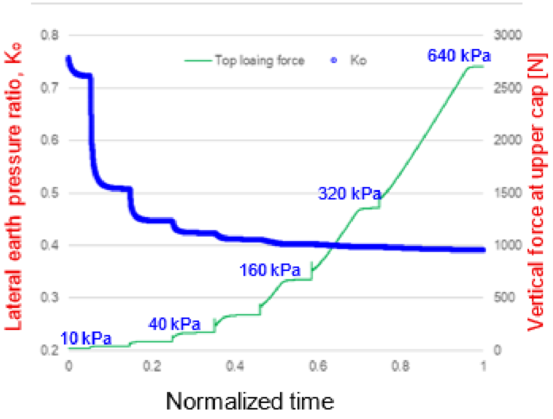


Fig. 5: Evolution of K_o during loading from 5 kPa to 640 kPa

0.761 and 0.732, respectively. K_o continuously decreases at a high rate from 0.732 to 0.431 during compression from 10 kPa to 40 kPa. The unstable value of K_o at this stage might be due to the relatively high void ratio of the specimen. Soil particles were quickly dislocated and rearranged. At heavy loading steps (from 80 kPa), K_o gradually decreases to approximately 0.397 at 640 kPa. The specimen might reach its well-confined state with a stable skeleton, resulting in a stable K_o value.

The decrease in K_o values indicates that the friction angle increases. By inverting the equation for K_o estimation (K_o = 1- sinφ), the friction angle (φ) is estimated to increase from approximately 14^o to 37^o. During loading, soil particles are rearranged by compression energy, which results in a compact specimen with high interparticle contacts. Therefore, the internal friction angle increases.

D. Contact force magnitude

The force chain at different loading steps was captured. Figure 6 illustrates the evolution of contact force chains in the DEM specimen under increasing vertical stress, ranging from 20 kPa to 640 kPa, during K_o-loading (i.e., constrained lateral strain) conditions. As the applied vertical stress increases, the magnitude and density of contact forces between particles also increase significantly. This is visually represented by the increasing thickness and brightness (intensity) of the force chains, typically depicted as cylindrical links between particles.

At light loading steps (20 kPa and 40 kPa), the contact force chains are sparse, weak, and evenly distributed, with mostly short, thin chains indicating a relatively loose packing and low interparticle force transmission. As vertical loading stress increases, the force chains begin to densify slightly, showing initial signs of preferential alignment and force concentration along vertical paths. At higher loading steps (320 kPa and 640 kPa), the vertical force chains are significantly more developed, longer, and thicker, indicating a well-formed internal force structure capable of efficiently transferring load. Force chains become densely packed and highly interconnected. Stronger and more continuous vertical chains dominate the specimen, representing high contact force magnitudes.

This evolution reflects the strain-hardening and fabric reorientation behavior of granular soils under one-dimensional compression. As the load increases, particles rearrange and mobilize stronger contact forces, resulting in a stiffer response and more pronounced anisotropy in force distribution.

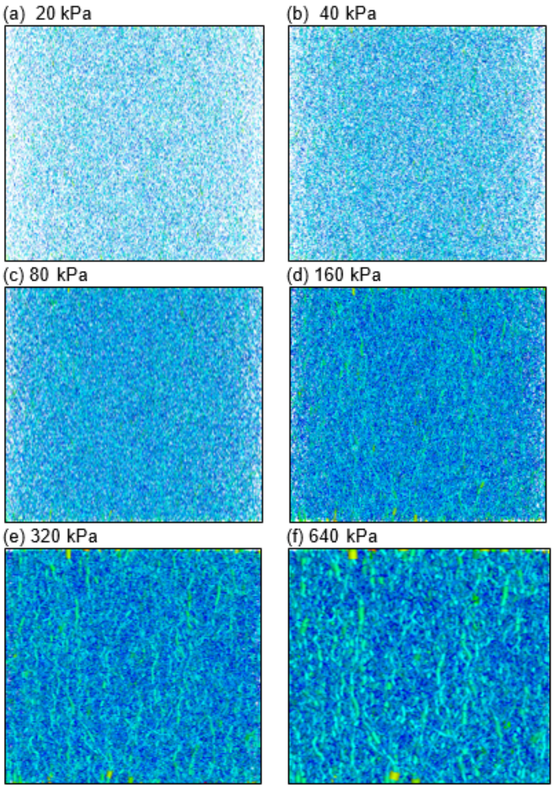


Fig. 6: volution of force chain during K_o loading condition, with the vertical pressures of (a) 20 kPa; (b) 40 kPa; (c) 80 kPa; (d) 160 kPa; (e) 320 kPa; (f) 640 kPa

V. CONCLUSION

The objective of this study is to investigate the macro- and micro-behaviors of soils with soluble particles by the DEM to simulate a conventional one-dimensional compression test on a soil specimen containing 10% salt by volume. In the model, salt particles are assigned substantially lower stiffness compared to sand particles. The 3D DEM simulation is validated against experimental data from a previous laboratory study. The oedometer test involves applying vertical loads ranging from 5 kPa to 640 kPa. Both macro- and micro-scale responses of the specimen are examined by monitoring parameters such as vertical strain, void ratio, vertical and horizontal stresses, and inter-particle contact forces during compression. From the simulation results, it was observed that the 3D DEM model closely replicates the laboratory findings, particularly showing a strong correlation between vertical strain and void ratio. Additionally, the lateral earth pressure ratio continuously decreased with increasing load, indicating that the internal friction angles increase during loading. Furthermore, force chain analysis reveals particle rearrangement and enhanced inter-particle interactions throughout the loading process.

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