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Discrete modelling of conventional triaxial tests

Modelado discreto de pruebas triaxiales convencionales

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ABSTRACT: This paper presents a comparative study between experimental and numerical results of conventional triaxial tests (CTT) simulated using Discrete Element Method (DEM). The contact properties between particles of the materials are calibrated. The granular material consists of 2902 steel balls with constant size both in the experimental and numerical tests. The triaxial cell is constituted by two horizontal rigid walls, upper and bottom, as well as a flexible lateral membrane represented by a hexagonal packing of bonded spheres. A linear and linear bond contact models are utilized for interactions between steel balls and membrane particles, respectively. The modelling includes generating a cylinder sample, applying isotropic compression, confining stress through the membrane boundary, and deviator stress. The load transmitted by the membrane is negligible when the normal and shear stiffness at the contact points fall within a range of 100 to 1000 N/m. A bond resistance of 10 MPa at the contact points of the membrane is sufficient for conducting the simulated tests. The laboratory experiments and numerical results shows a good agreement despite the limited number of particles constituting the samples. A frictional coefficient equal 0.10 in the interaction between the steel balls samples was used.

KEYWORDS: DEM, Conventional triaxial test, flexible membrane, steel balls samples, frictional coefficient

1 INTRODUCTION

The mechanical characterization of soils has led to development of various tests: triaxial test, direct shear test, deformability test, among others. The triaxial test involves placing a cylindrical sample between two horizontal plates in a chamber. The sample is covered by a flexible membrane. Two porous rocks are positioned between the sample and plates, to allow for the drainage and saturation of the material. The confinement stress is applied through a pressurized fluid. The shearing of the sample is induced by applying an axial load using controlled deformations of sample. Pressures within the chamber are recorded, enabling the determination of shearing strength, compressibility, and deformation capacity of soils. Several types of tests are used with different drainage conditions: Unconsolidated-Undrained (UU), Consolidated-Undrained (CU), Consolidated-Drained (CD), Drained (D).

The advantage of the compression triaxial test is that volumetric variation of specimen and the pore pressure are monitored. However, experimental works provide limited elements for understanding the mechanics that govern the overall behaviour of soil. Some researchers have applied sophisticated techniques to explore the inner mechanical phenomena that occur during the execution of a triaxial test. Fu (2005), Mohmad and Dayakar (2020) and Xiang *et al.,* (2021) examined the micro-mechanical behaviour of granular materials, using X-ray and mechanical tests. This technique offers interesting results, but it involves a significant economic and time effort and can be strongly affected by the geometric scale effect (Auvinet and Bouvard, 1984). An alternative is the use of the computational and mathematical models that allow modelling the real problem. These models permit assessing the mechanical behavior of granular media both at the global and particles level.

The DEM proposed by Cundall (1971) is an important tool for studying granular materials. DEM has been used for modelling experimental geotechnical tests, allowing the analysis of the inner structure and micromechanical behaviour of granular materials. The CTT modelling is important because this test is the most widely used. Different methodologies have been suggested to reproduce the boundary conditions of this test with DEM.

Cundall (1989), Bardet and Proubet (1991) and Wang *et al.,* (2017) employed periodic boundary conditions. This technique aims to control the displacements of particles located on the outer surface of the sample. Thornton (2000) points out that this method ineffectively maintains the confinement stress during the deviator load applications.

Kuhn (1995) proposes a flexible membrane that incorporates particles furthest from the centre of the sample. These particles are submitted to confinement forces along the boundary. Cheung and O'Sullivan (2008) and O'Sullivan and Cui (2009) use the same criteria; however, they employ a Voronoi diagram to identify the outermost particles. The disadvantage of these techniques is that the boundary remains cylindrical in shape during shearing (Mohammad *et al.,* 2018). A practical alternative and commonly utilized method involve implementing a flexible boundary composed of constant-size spheres, with contacts allowing for bonding strength but with zero bending force. de Bono *et al.,* (2012), Cil and Alshibli (2014), Lu *et al.,* (2018), Qu *et al.,* (2019), Pham *et al.,* (2021), Wu *et al.,* (2021) and Li *et al.,* (2022) have pointed out that this method provides a good approximation to numerical and experimental results. Additionally, it allows for the exploration of different types of failures.

This study presents the calibration of contacts parameters that are required for modelling a CTT using a flexible membrane in DEM. The boundary conditions were considered based on previous studies conducted by Qu *et al.,* (2019), Li *et al.,* (2022) y Wu *et al.,* (2021). Experimental data from a series of CTT on steel balls samples were utilized for calibration.

2 EXPERIMENTAL TESTS

A series of CTT on steel balls samples was conducted in the laboratory. For this purpose, three different levels of confinement stress were considered, and the stress-deformation behaviour, as well as the internal friction angle were measured. The test specimens were prepared in a cylindrical container with a diameter of 3.6 cm and height of 8 cm. A triaxial testing apparatus named SBEL was used, which consists of a hydrostatic load cell, an LVDT (Linear Variable Differential Transducer) for measuring displacements and pressure sensors. The steel balls sample with particles of diameter equal 3.18 mm and a specific gravity of 7.68 were positioned in the load cell. The particles were carefully introduced in the cylindrical container using a funnel. A stress suction was applied to stabilize the specimens and the confinement stress (σ_3) was applied using liquid pressures of 50, 80 y 120 kPa, respectively. The deviator stress was applied at a rate of 0.60 mm/min until a 20 % axial strain (ε_a) was attained. The characteristics of the specimens are presented in Table 1.

Table 1. Characteristics of the steel balls samples

Sample	*1*	*2*	*3*
Diameter [cm]	3.62	3.60	3.63
Height [cm]	8.00	8.00	8.00
Unit weight, γ_d [kN/m^3]	44.93	45.43	44.68
Porosity, *n*	0.406	0.399	0.409

In Figure 1, the strain-stress behaviour, measured experimentally for the steel ball samples subjected to triaxial compression test is presented. The irregularities in the stress-strain curves suggest that the dimensions of the balls are too large relative to the size of the samples, which implies visible internal local structural changes in the material, leading to sudden decreases and increases in load. The issue of geometrical scale effect in granular material samples, has been studied by Auvinet and Bouvard (1984) and Auvinet and Sánchez (2023).

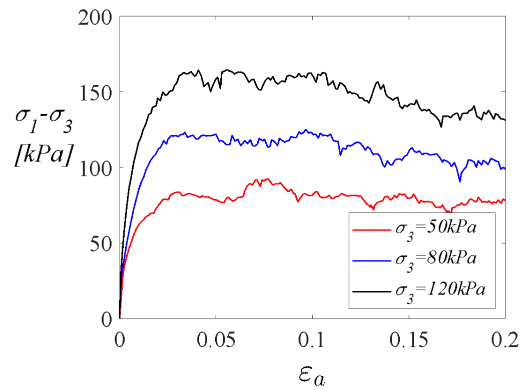


Figure 1. Experimental stress-strain behavior of a steel balls samples

3 NUMERICAL MODELLLING OF CTT

The simulation of a CTT using flexible boundary was implemented in PFC3D (Itasca, 2018). The steel balls cylindrical samples were represented by an arrangement of spheres using the same number and dimensions of particles as those used in the laboratory test. The methodology consists of five steps: sample generation, isotropic compression, construction of the membrane, application of confinement stress and shearing. The features of each of these steps are described below:

a) Sample generation: The specimen is created within a cylindrical wall limited by two horizontal upper and lower plates. The particles are placed into the cylindrical wall, simulating the effect of the funnel used in the laboratory. A linear contact model (LCM) is considered for modelling the interaction between steel balls (Fig. 2a) and allowing the particles to separate and join due to the acting force. The parameters include interparticle frictional coefficient (μ), damping coefficient (β), normal stiffness (k_n) and tangential stiffness (k_s). The interaction between the balls and the wall follows the same contact model. The initial state of the sample is simulated by applying cycles of calculations until equilibrium is achieved (Fig. 3a).

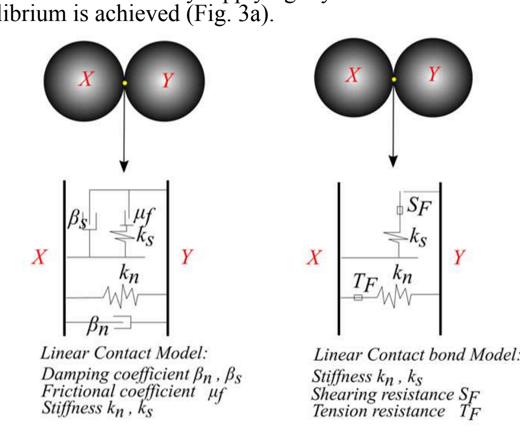
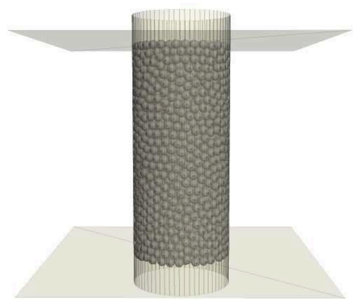


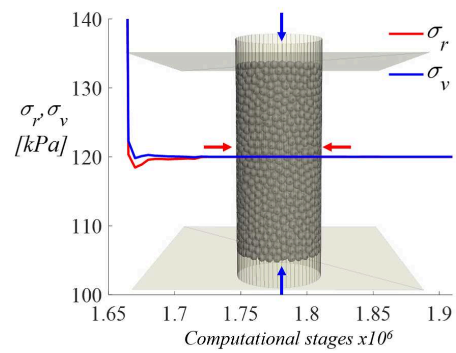
Figure 2. Rheology of the contact model a) LCM and b) LCBM

b) Isotropic stress application: The sample is subjected to a state of isotropic stress by servo-controlling the upper, lower, and lateral walls. Cycles of calculation are applied until the stress in the walls reaches the prescribed confinement stress (Fig. 3b).

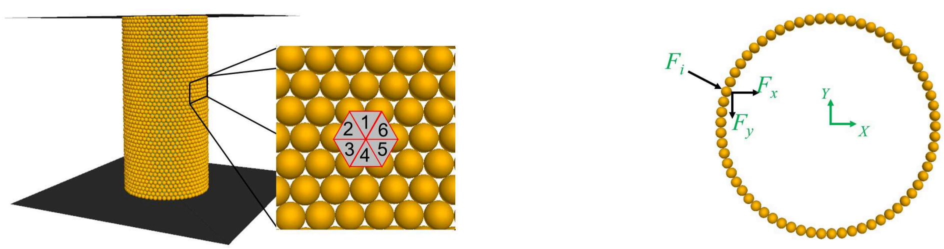
c) Flexible membrane installation: The boundary conditions of a triaxial test can influence the type of failure observed in the material. To simulate the flexible membrane in DEM, the methodology provided by de Bono *et al.,* (2012), Qu *et al.,* (2019), Wu *et al.,* (2021) and Li *et al.,* (2022) is employed. In this process, the cylindrical wall is removed, and a set of constant-size particles is used to construct the cylindrical flexible membrane (Fig. 3c). These particles are arranged in a closed hexagonal pattern which helps minimizing particle flow through the membrane (Li *et al*., 2022). Qu *et al.,* (2019) determined that a ratio between diameter of sample and membrane spheres ranging from 35 to 120 allows achieving results with error of less than 5% on the stress-strain behaviour. The pores among the membrane particles must prevent the escape of elements of granular medium. The flexible membrane is modelled using the linear contact bond model (LCBM) (Figure 2b). This implies that strong bonds, but no bending force, develop between particles. The parameters involved are normal stiffness (k_n), tangential stiffness (k_s) and bonding strength in both normal (S_F) and tangential direction (T_F).



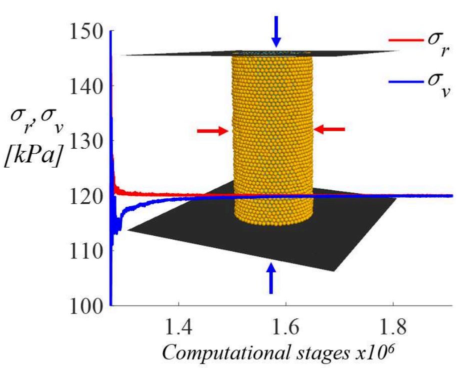
a) Sample generation



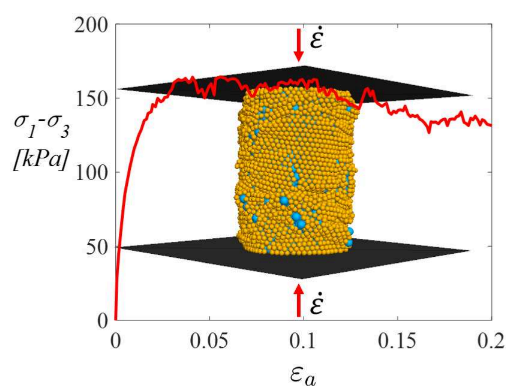
b) Isotropic compression



c) Construction of membrane



d) Confinement stress application



e) Stress deviator application

Figure 3. Step for modeling a Conventional Triaxial Test using DEM

d) Confinement stress application: Application of the confinement stress is achieved through discretization by means of triangles with vertices located at the centres of membrane particles. The hexagonal arrangement induces six areas adjacent to each sphere (Fig. 3c). The resultant force directed toward the centre of the sample can be calculated based on those areas (see Eq.1). This criterion ensures that the force remains compatible with the deformation of the membrane in the different calculation cycles. A set of calculations is carried out to verify the convergence of radial stress (in membrane particles) with the vertical stress (in the upper and the lower plates) (Fig. 3d).

$$F_i = \sigma_3 \sum_{1}^{6} n_i A_j \quad (1)$$

F_i: resultant force in membrane particle i; σ_3: confinement stress; n_i: normal vector of area j and A_j: area of element j.

e) Stress deviator application: This step involves applying a load by moving the upper plate downward and the lower plate upward. This process is applied until a 20% axial strain is attained. The deformation rate during the load application is calculated considering the system as quasi-static with an inertia factor (I) equal to 0.0001 (see Eq. 2).

$$I = \dot{\varepsilon}\sqrt{\frac{m}{\sigma_3 d}} \quad (2)$$

I: inertia factor minor than 10^{-4}, $\dot{\varepsilon}$: deformation rate, m: mass of steel balls, d: diameter of steel balls and σ_3: confinement stress.

The major principal stress (σ_1) is determined by dividing the applied force on the walls by the cross-sectional area of the sample. Deviator stress is calculated as the difference between the major principal stress and the confinement stress (σ_3). The unit axial strain (ε_a) is calculated from the initial (h_0) and final (h) heights of the specimen.

3.1 PARAMETERS OF NUMERICAL MODEL

3.1.1 *Parameters of the flexible membrane*

The challenge with the methodology presented lies in assigning representative contact parameters to the flexible membrane. Qu *et al.,* (2019) have provided equations for determining k_n and k_s. However, these parameters largely depend on the stress conditions; it is therefore advisable to conduct a calibration to assess the effects of the flexible boundary on the mechanical behaviour of the tested granular material (Li *et al.,* 2022).

The determination of contact parameters between particles of the membrane was carried out with the prerequisite that these parameters should be kept sufficiently low to minimize the load transmitted to both the upper and lower plates. de Bono *et al.,* (2012), Qu *et al.,* (2019), Wu *et al.,* (2021) and Li *et al.,* (2022) suggest that k_n and k_s lie between 100 to 1000 kN/m and the bonding strength must be major that 10 MPa.

A simulation of CTT was conducted to confirm the stiffness in the contact between membrane particles, considering a k_n/k_s ratio of 1.0 with values equal to 500 N/m and a bonding strength equal to 10 MPa. The simulations were performed under a confinement stress of 120 kPa and the force on walls of steel balls and membrane was measured. Figure 6 shows the contribution of the flexible membrane to the stress-deformation behaviour. This contribution may be negligible for k_n and k_s values equal to 500 N/m.

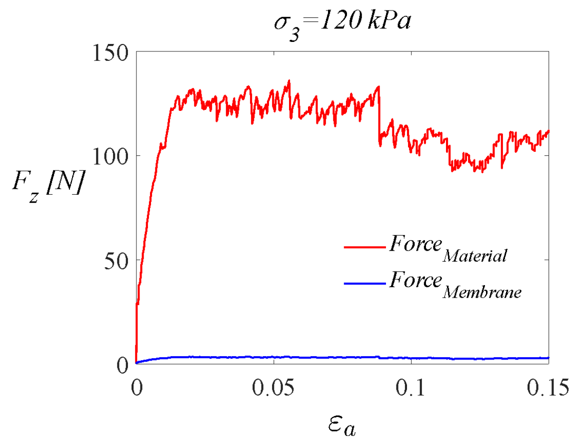


Figure 6. Contribution of flexible membrane to the stress-strain behaviour

3.1.2 *Parameters of steel balls*

The effect of the contacts properties of a specimen of steel balls subjected to triaxial stress on the stress-deformation behaviour was studied. A set of simulations of CCT was conducted, considering various values of frictional interparticle coefficient (μ), as well as of normal (k_n) and tangential (k_s) stiffness for steel balls. This analysis involves modelling a CCT using the methodology described in section 3. Dimensions of specimen were approximately 80 mm in height and 36 mm in diameter. The sample consisted of 2902 spheres, each with a diameter of 3.20 mm and k_n=k_s=10^7 N/m at their contacts. which closely matched physical samples. An isotropic compression of 120 kPa, which corresponds to the confinement stress applied in the laboratory triaxial test, was applied using a servo control.

The flexible membrane was constructed as shown on Figure 3c, with a diameter ratio between the sample´s steel balls and the membrane particles equal to 40. The normal and tangential stiffness at the particles contacts of membrane were equal to 500 N/m, with a bonding strength of 10 MPa. The deviator stress was applied until the specimen has achieved an axial strain ε_a = 20%.

A set of the simulations was conducted, considering different values of μ ranging from *0.10* to *0.70*, with constant value of normal and tangential stiffness of 10^7 N/m for the contacts among steel balls. Figure 7 presents the effect of the interparticle frictional coefficient on stress-strain behaviour, indicating that the strength of granular material is directly proportional to μ.

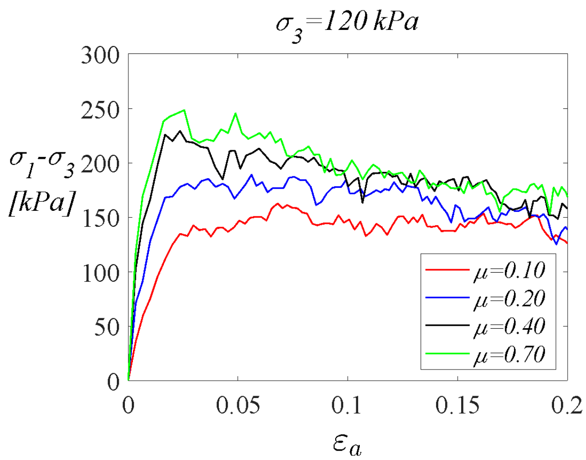
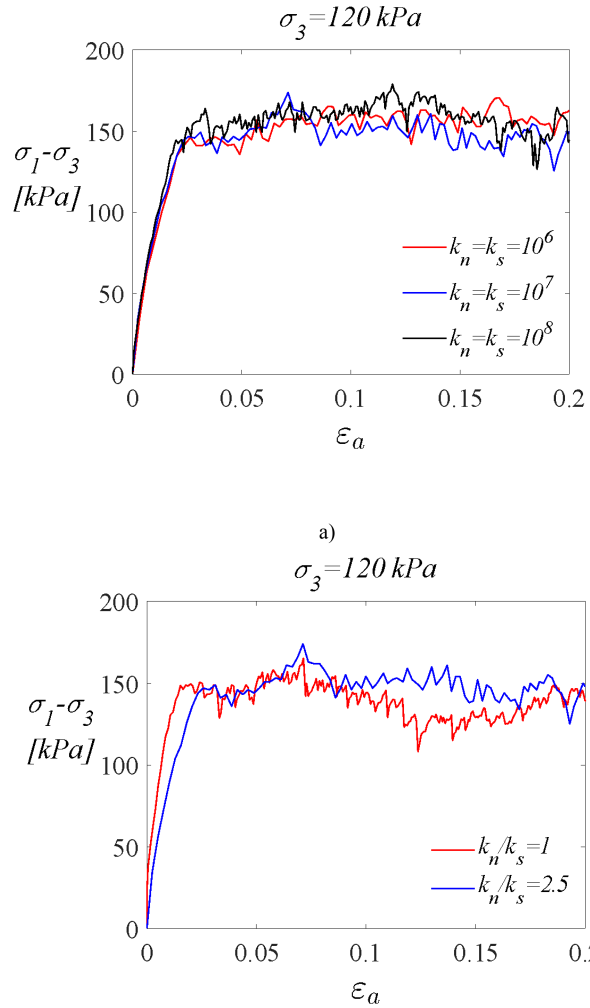


Figure 7. Effect of inter-friction coefficient on stress-strain behaviour

Another set of simulation was conducted considering a variation of both normal and tangential stiffness at the contact points between the steel balls. A constant value of μ at 0.1 was used. The stiffness values considered ranged from 10^6 to 10^8 N/m with a k_n/k_s ratio equal to one. Additionally, the effect of k_n/k_s was analysed by considering values of 1 and 2.5. Figure 8a shows the influence of the variation of normal and tangential stiffness on the stress-deformation behaviour of a steel balls sample. It is observed that the effect of stiffness at the contact points between the particles on the stress-deformation behaviour is negligible. However, an increase in the ratio k_n/k_s leads to a smaller slope at lower deformations (Fig. 8b), which confirms the findings by Hazzar *et al*., (2020). This effect is due to the higher stiffness in the normal direction at the particles contacts that conducts to an unbalanced contact force and greater deformation in the tangential direction. This phenomenon contributes to a reduction in the elastic modulus of the granular media.



b)

Figure 8. Effect of contact stiffness on the stress-strain behavior of particles assemblies. a) $k_n=k_s$ b) variation of k_n/k_s

3.2 VALIDATIONS OF THE NUMERICAL RESULTS

3.2.1 Characteristics of modelling

The simulations of a CTT on specimens of steel balls in DEM were carried out using PFC3D v5 (Itasca, 2018). The dimensions of simulated sample were 80 mm in height and 36 mm in diameter, consisting of 2902 constant-size particles measuring 3.20 mm each. The normal and tangential stiffness of contact point between particles were set at 10^7 N/m. Additionally, a μ value of 0.10 was used based on the sensitivity analysis (Fig. 7). The confinement stress considered was equal to 50, 80 y 120 kPa which closely matched laboratory triaxial tests. The flexible membrane was constructed according to section 3, with a diameter ratio between the sample´s steel balls and the membrane particles equal to 40.

Table 2. Characteristics of the steel balls samples

Properties	*Wall*	*Ball*	*Membrane*
k_n, k_s [N/m]	10^7	10^7	500
μ	0.0	0.10	0.0
S_F, T_F [MPa]	-	-	10

The porosity was evaluated using the Monte Carlo technique, which involves generating random points in space and recording those that fall within the porous areas. Auvinet and Sánchez (2023) recommended using 10^7 or more random. Porosity (n) is calculated as the ratio of the number of points within the porous areas to the total number of points. The standard deviation of porosity was evaluated. Auvinet and Bouvard, (1984) proposed an expression, which is function of porosity, specific grain surface (S_3) and central measuring cube.

$$\frac{\sigma_n}{\sqrt{n(n-1)}} = 1.4\left[\frac{aS_3}{4n(1-n)}\right]^{-\frac{3}{2}} \quad (3)$$

Where:
σ_n: Standard deviation of porosity
a: edge of central measuring cube

$$S_3 = \frac{3}{2n} E_{3V}\left\{\frac{1}{d}\right\} \quad (4)$$

d: diameter of particle sample
E_{3V}: mean value of the inverse grain diameter

Auvinet and Bouvard (1984) suggest using value equal to a=4.5d to eliminate the boundary effect in the measuring of porosity. Table 3 compares the experimental and numerical porosity values of fabric samples.

Table 3. standard deviation of Porosity

Sample	n	σn
Experimental	0.4046	$9.55\text{x}10^{-3}$
Numerical	0.4006	$9.33\text{x}10^{-3}$

The confining pressure was applied using a membrane of particles (Fig. 3c). The particles in contact with the upper and lower plates were assumed to have zero lateral displacement. Deviator stress was applied until the axial strain reached 20%.

4. COMPARISON BETWEEN NUMERICAL MODEL AND EXPERIMENTAL RESULTS

The DEM simulation results were fitted to the experimental curves, using the parameters reported in table 2 for confining pressures of 50, 80 y 120 kPa. Figure 9 shows that the stress-deformation behaviour obtained from numerical tests is consistent with the results obtained from laboratory tests for each confining pressure. However, it is important to mention that the size of the samples lacks representativeness, which can influence the exact coincidence of the numerical and experimental results. To improve the results, especially for significant deformation levels, it would be necessary to maintain the same conditions in both situations, including the number and precise positioning of the particles. Otherwise, it is necessary to provide a set of numerical and experimental tests using diverse samples to establish the possible range of results.

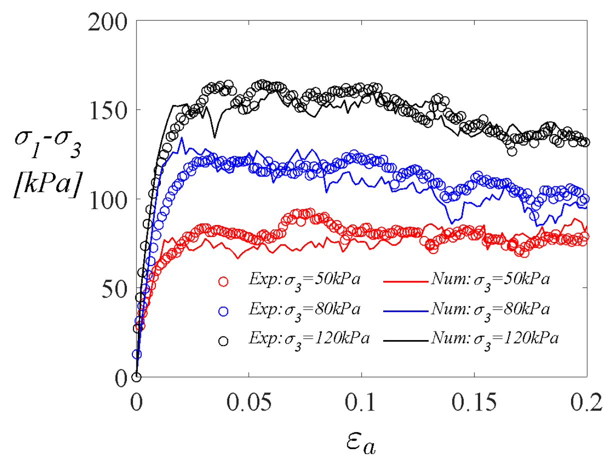
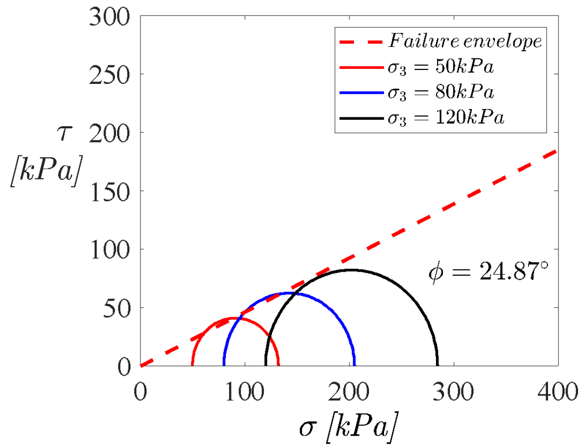


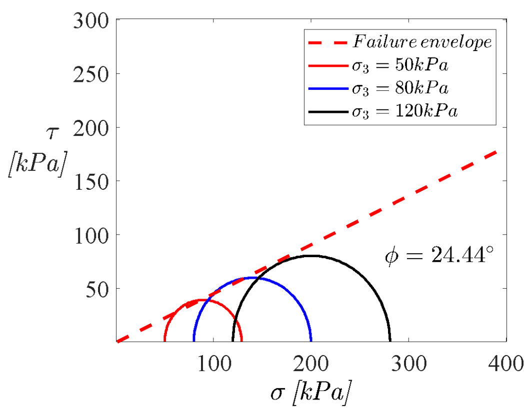
Figure 9. Comparison of experimental and numerical stress-strain behavior.

The Mohr-Coulomb criterion was used to determine the frictional internal angle (φ) of the steel ball samples tested both experimentally and numerically. Figure 10 shows the Mohr circles of a sample subjected to triaxial stress, obtained from both numerical and experimental data. In both cases, a φ value of 25° was obtained. This coincidence shows that the behavior of steel ball samples can be replicated with DEM.

Conversely, it is observed that φ =25° corresponds to μ =0.45, indicating that the granular fabric makes a considerable contribution to macroscopical strength of granular medium (Auvinet and Sánchez, 2023). The failure envelope curve is not secant to the three Mohr circle, indicating that the steel ball sample exhibits dilation. This is likely due to the rearrangement of particles under low stresses confinement, which confirms the findings by Bishop (1972).



a)



b)

Figure 10. Comparison of frictional internal angle of a steel ball sample determined experimentally (a) and numerically (b).

3 CONCLUSIONS

In this study, a methodology was developed to simulate a Conventional Triaxial Test with DEM. It was possible to simulate a CTT by considering a flexible membrane composed of constant-size bonded spheres.

The parameters of contact particles for simulating a flexible membrane were identified. The results suggest a stiffness for these contacts varying from 100 to 1000 N/m, ensuring that the load transmitted to the flexible boundary is minimal. A bonding strength in these contacts greater than 10 MPa provides stability from a numerical standpoint.

Regardless of the lack of representativeness of steel balls sample due to the limited number of particles, the numerical and experimental results showed good agreement. A frictional interparticle coefficient of 0.10 proved to be suitable for simulating the mechanical behavior of a steel balls sample with DEM.

This study shows the utility of DEM for simulating a Conventional Triaxial Test, which provides the benefit of studying the behavior of granular materials at the particle level under various load conditions.

This research has served as the foundation for a geotechnical investigation focusing on the mechanical behavior of volcanic scoria samples with a greater number of particles and diverse grain-size distributions.

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