FINAL REPORT

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1. INTRODUCTION

Brief and concise information about the research work carried out within the framework of the BAYLAT 2019 scholarship is presented in this report, which took place during 5 months from February to June 2020 at the Technical University of Munich under the supervision of Prof. Dr. Ing. Roberto Cudmani and Dr. Ing. Andrés Peña Olarte.

1.1. OBJECTIVES

Numerical simulations using the discrete element method (DEM) have become a valuable tool and cost-effective way of studying the loading response of granular soils, as it enable the understanding of complex material behavior. DEM enables to simulate discontinuous nature of granular materials by discretizing the space into discrete particles. Furthermore, DEM allows studying, following and understanding phenomena occurring at the particle level, this allows to correlate in detail the macroscopic stress-strain response with the underlying micro-mechanical phenomena.

The main objective of this work is to carry out numerical simulations of geotechnical tests by means of the discrete element method: in particular to be able to represent the mechanical response of Karlsruhe Fine sand, proposing a sample preparation procedure and carrying out drained triaxial tests to understand the effect and calibrate the micro-mechanical parameters of the contact law using as reference the experimental database for the sand. In addition, the application of cyclic loading in two dimensions was studied to evaluate the dynamic behavior of granular assemblies.

1.2. ACTIVITIES OUTLINE

A brief description of the activities carried out by the student during the research period is presented below as they will be described in the subsequent sections of this report:

In **Section 2**, the Discrete Element Method (DEM) is introduced. A comprehensive study of the numerical formulation of the method was carried out. The numerical sequence in simulations and the two contact models used in this study are presented.

In **Section 3**, a contact law parameters calibration process is done by means of the DEM, validating the method to successfully represent the mechanical response of real materials. In this case the material to be calibrated is Karlsruhe Fine sand, taking as reference the experimental database developed by T. Witchmann [1]. This section is divided into two main parts. First, the samples preparation process with specified relative densities is described. In order to compute relative density of samples, the maximum and minimum void ratios of the samples (e_{max}, e_{min}) are computed using isotropic compression. In the second part, drained triaxial tests are carried out to compare the results with experimental data. Parametric studies are conducted to understand the effect of different micro-mechanical contact law parameters on the macroscopic behavior of the sand. Finally, calibrated contact law parameters are presented for Karlsruhe sand, along with graphs with the resulting calibration for dense samples.

In **Section 4**, dynamic analyzes with the DEM is carried out. First, a theoretical framework is described, previous investigations regarding liquefaction phenomena of granular soils by several authors is presented. Cyclic biaxial tests with stress and strain cycles are simulated to study the dynamic behavior of granular assemblies. Stress path and hysteris loops are presented in correspondence with what was obtained by researchers.

Finally in **Section 5** some remarks and conclusions are provided.

2. DISCRETE ELEMENT METHOD

The Discrete element method (DEM), was first introduced by Cundall and Strack in 1979, in which particles were modelled as an assembly of two dimensional disks and interaction of particles was monitored through all contacts and the motion of particles was modelled particle by particle [2] . As the DEM developed, complex geometries and complex contact algorithms were implemented, both in 2D and 3D, enabling to model mechanical behavior of granular assemblies. Today DEM is widely accepted as an effective method of addressing engineering problems in discontinuum materials.

Despite advantages, DEM is computationally challenging. The maximum number of particles and the duration of a virtual simulation are limited by computational power.

In the last decades, a number of softwares have been developed for DEM. Yade (Yet Another Dynamic Engine) is an extensible open-source framework for discrete numerical models, focused on discrete element method. The computation parts are written in c++ using flexible object model, allowing independent implementation of new algorithms and interfaces. YADE is used in this study due to its basic nature along with extensive documentation/trouble shooting through the forums on their website (yade-dem.org). [3]

2.1. DEM FORMULATION.

A typical DEM simulation starts by first generating a model, which results in creating and spatially orienting all particles. As the particles (spheres, polyhedral, etc.) interact at contacts according to simple physical laws, and a finite difference (time-stepping) algorithm is settled, the imbalances in the forces on each particle impel the particles into new positions with each time step by solving Newton's equations of motion. Generally, a simulation consists of three parts: the initialization, explicit time-stepping, and post-processing.

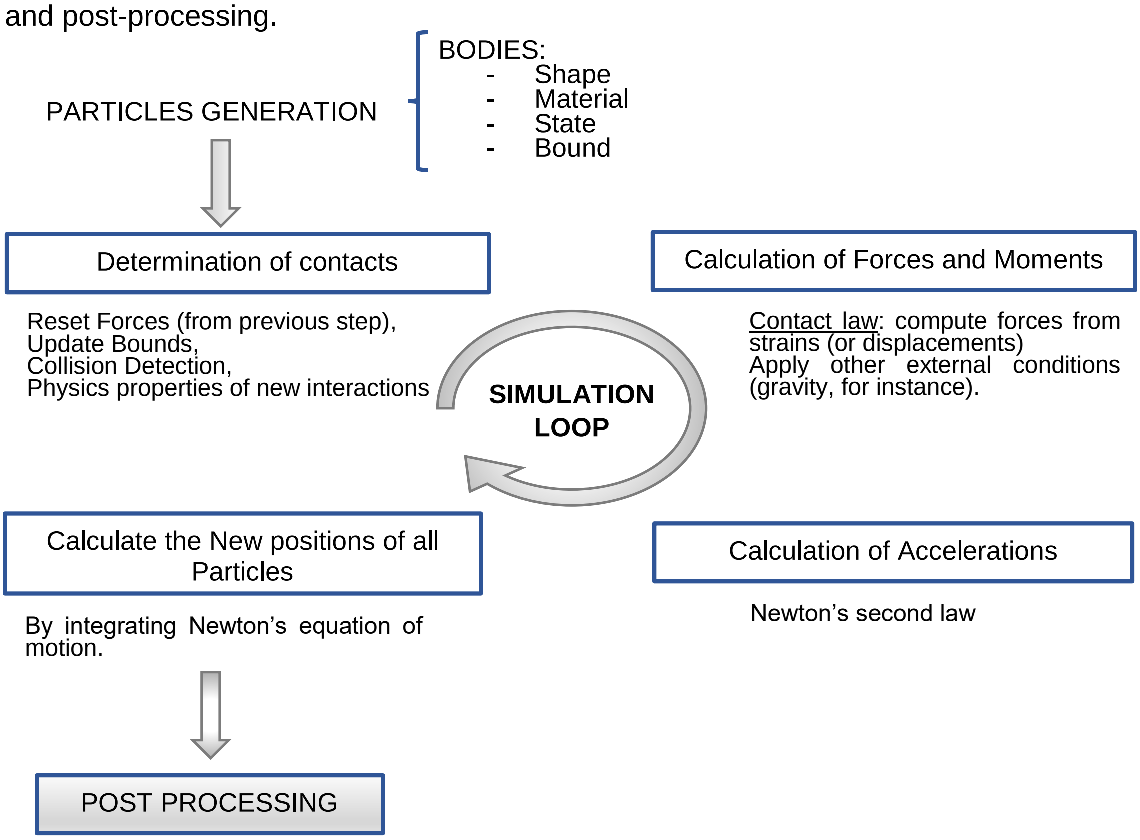


Fig. 1: Typical simulation scheme with calculation sequence.

Once the particles have been created, the most challenging part is to detect the contacts between the particles during each iteration. Collision detection depends on the geometrical overlap of the particles, but there are also non-geometrical properties of the interaction to be determined, those that have to do with the material type of both particles interacting. Collision detection algorithms for collision of two spheres or other combinations run at every time step since it is at every step that particles can change their mutual position.

In the general case, considering two spheres that enter into contact, the force between the particles can be then resolved into two component, one in normal direction and one in tangential direction. The forces acting on both spheres are computed using contact models in DEM, also known as *contact laws*. It is possible to find a great variety of constitutive models of contact between particles from simple elastic laws to complex laws of union with cohesion and rotation. Once the contact law parameters are defined and all the interactions follow the same frictional law, normal and tangential force vectors can be computed.

In this research work, the two main simple contact laws used are: **linear elastic with simple friction** and **linear elastic with simple friction and simple rotation**.

The first one is one of the simplest contact laws defined by Cundall and Strack [2] for materials without cohesion and requires four material parameters which are: contact stiffness (E_c), Poisson or contact stiffness ratio (ν_c), contact friction angle (ϕ) and density (δ). Iwashita and Oda [4] modified the linear elastic law such that the effect of rolling resistance at contacts could be taken into account. Two rotational parameters are added along with the four presented before: rotational stiffness (k_r) and rotational coefficient (η).

3. MATERIAL CALIBRATION

In order to perform numerical tests on a specific granular material, it is important to calibrate the underlying contact law with laboratory tests results, simple experiments are commonly used as reference for this task. Regardless of the experiment, the calibration is performed by a systematic variation of the parameters of an existing model, in an iterative process of trial and error, until the desired behavior is well represented.

In this study the contact parameters were calibrated using the corresponding drained triaxial tests with monotonic loading experimentally conducted on Karlsruhe Fine sand by T. Witchmann and Th. Triantafyllidis [1].

The following five material parameters are needed for the contact law calibration: contact stiffness E_c, contact stiffness ratio ν_c, contact friction angle ϕ, rotational stiffness k_r and rotational coefficient η. In YADE, simple linear rotational moment law between spheres is introduced to increase the rolling resistance and take into account the particle shape and roughness.

The radii of particles in DEM are assigned following the up-scaled particle size distribution of Karlsruhe Fine sand given in Fig.2 to avoid computation times becoming very high due to small radius values.

The whole simulation process was separated into two parts. In the first part, a cloud of particles was created and then isotropically compressed to the required confining stress under gravity-free conditions. In the second part, shearing is done by axial strain application with a sufficiently slow strain rate to ensure quasi static conditions. Damping coefficient is kept at a low value of 0.2 to maintain the numerical stability of the method, yet large enough to obtain a quick convergence to a quasi-static state of equilibrium of the assembly and reduce computational time.

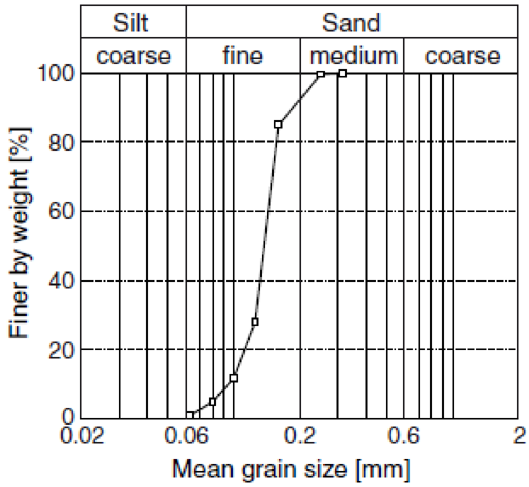


Fig. 2: Tested grain size distribution curve [1]

3.1. SAMPLE PREPARATION

To be able to calibrate the, the simulated samples must be meaningful comparable with the samples from Karlsruhe sand experiments, in terms of confining pressure and void ratio (microstructure). Creating a sample at an exact void ratio corresponding to the given relative density is challenging. The complexity lies in grain morphology. When the shape of the particles for both experimental and numerical methods are comparable, as is the case of rounded sands where the shape of the particle can be idealized as spherical particles, it is possible to reproduce specimens with a similar void ratio. In the case of Karlsruhe sand, which has a sub-angular shape and is represented with spherical particles, to ensure creation of alike samples in terms of particle-void configuration, the parameter used as a guide to compare the behavior of experimental and numerical samples is relative density, given as:

$$ID_0 = (e_{max} - e_0)/(e_{max} - e_{min}) \quad (1)$$

The minimum and maximum void ratios from database e_{min} and e_{max} were determined from standard tests (at mean pressure $p = 0$). The initial void ratio e_0 was measured at the initial pressure p_0 of a test.

3.1.1. Maximum and minimum void ratios

An attempt has been made in this study to obtain maximum and minimum void ratio by means of isotropic compression using 'TriaxialStressController' engine in YADE. Isotropic compression is a widely used method in literature to prepare samples in DEM. Although it does not correspond to the standard ways to find the material's maximum and minimum void ratios, these parameters were commonly defined based on the response of the assembly subjected to isotropic compression. This is achieved by setting the friction angle during the compression phase to a low value in the case of the densest state, and a high value for the looser state.

A series of isotropic compression tests were performed to obtain the limiting void ratios (e_{max}, e_{min}), and subsequent be able to compute the relative density of the samples as in equation (1). For initial analysis, contact stiffness is set to $5e^8$ Pa, contact stiffness ratio of 0.1, the friction angle is varied from 0° to 60° and density of 2660 kg/m^3 was considered. Parametric studies were carried out to evaluate the effect of number of particles (sample size) and contact friction angle during isotropic compression.

3.1.2. Sample preparation for subsequent Triaxial Test

A cloud of 8000 (this is considered a suitable sample size to avoid boundary effects based on previous analyzes) no overlapping spheres is randomly generated in a cubical gravity-free space surrounded by rigid boundaries.

In a second step, the contact friction angle is set to prepare samples of various relative densities and the assembly is subjected to isotropic compression. This can be done by controlling the wall stresses or by a growing particle process until the predetermined confining pressure is reached (100 kPa, 200 kPa and 300 kPa). Fig. 3 shows the sample prepared before shearing.

Since parametric studies are intended in the calibration process, it is important to keep constant properties of the fabric (initial position and properties of the particles) during the testing program. For this reason, once the sample has been prepared for a given confining stress, the geometric properties for each body (global coordinates, particle radius) are exported to a text file. When needed, this text file is imported into another simulation using the 'Omega.load' function to create a sample of exact same porosity and given confining stress and test it as many times as necessary.

3.2. TRIAXIAL TESTS

Simulation of triaxial tests with DEM was used by many researchers for the calibration of the numerical material in order to match the material response of sands. Some examples can be mentioned: Widulinski et al. [5] carried out simulations of drained triaxial tests in 3D model of spherical particles in YADE, including rolling resistance to take into account the roughness of the grain, studied the effect of different components of the contact law on stress-strain behavior and compared with sands laboratory test results. Kozicki et al. [6] used a 3D model in YADE as well, to conduct quasi-static drained triaxial compression tests on cohessionless sand, the irregular grain shape was modelled as twelve different symmetric clusters of rigid spheres and compared with experimental results. .

Based on this theoretical guideline, three-dimensional drained triaxial tests were simulated to calibrate the contact law micromechanical parameters to represent Karlsruhe Fine sand's behavior. The calibration is done by carrying out a parametric study of these parameters (contact stiffness E_c, contact stiffness ratio ν_c, rotational stiffness k_r and rotational coefficient η) separately and comparing the results of triaxial test with the corresponding experimental results from database.

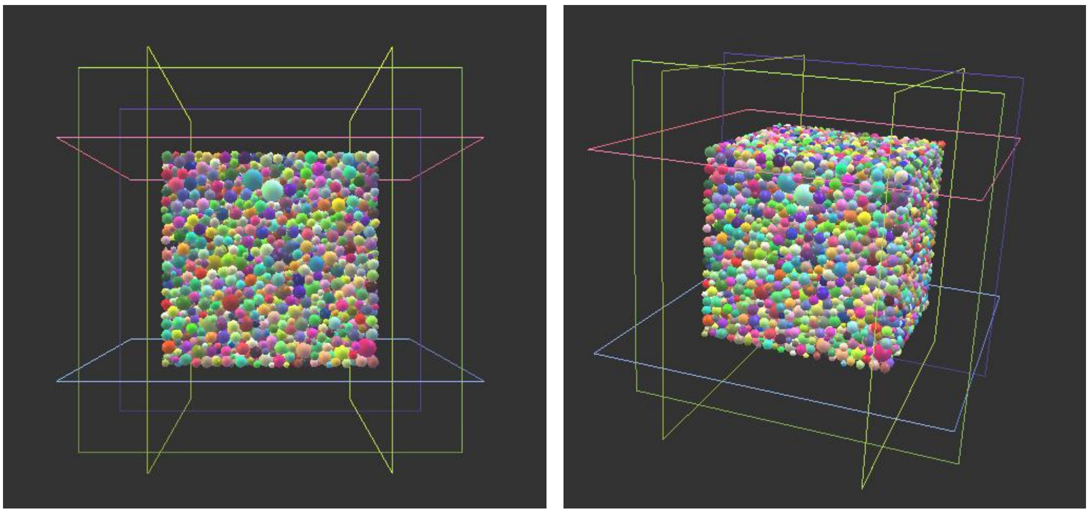


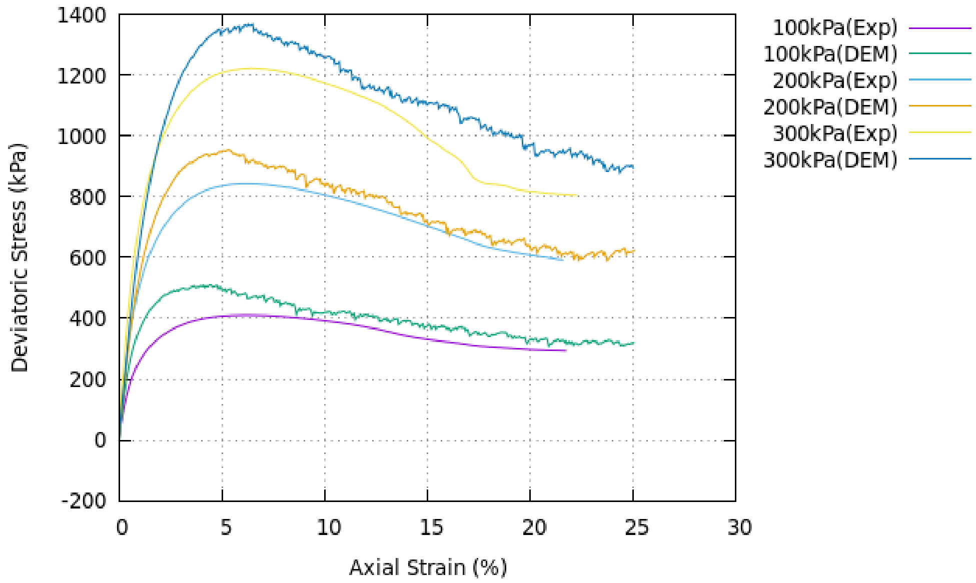
Fig. 3: Final prepared 3D sample with rigid boundaries.

3.2.1. Contact parameters for Karlsruhe sand

The numerical results of triaxial tests on dense samples were directly compared with the corresponding results of triaxial tests performed by Witchmann[1]. This test were done at confining stresses of 100kPa, 200kPa and 300kPa. Fig.4 shows the comparison of numerical behavior with experimental results. Both experimental curves (deviatoric stress versus axial strain and volumetric strain versus axial strain) are reproduced very well. Table 1 summarizes the calibrated parameters for Karlsruhe Fine sand.

Contact law Parameter	Values
Contact stiffness E_c	$5e8\ Pa$
Contact stiffness ratio ν_c	0.1
Rotational stiffness k_r	0.15
Rotational coefficient η	0.5

Table 1: Calibrated contact parameters for Karlsruhe sand.



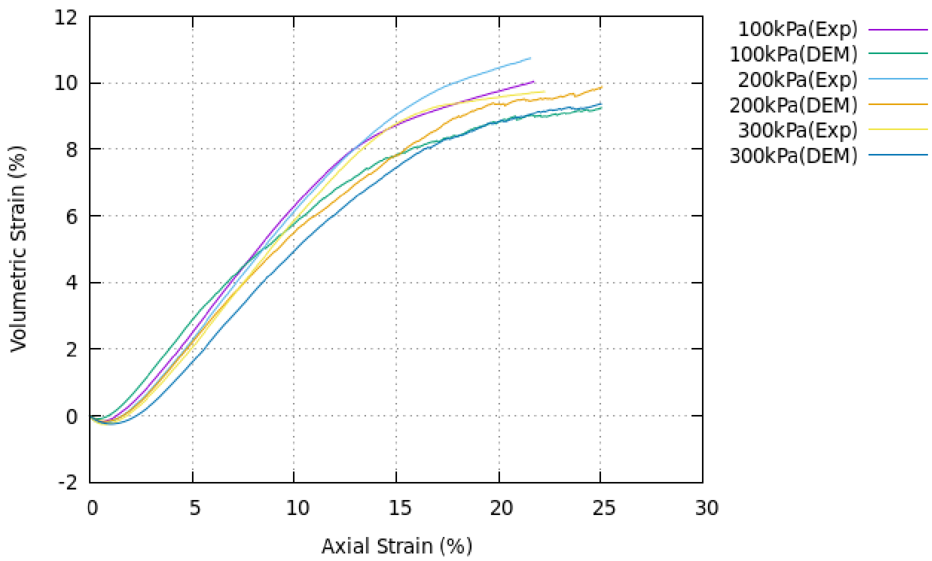


Fig. 4: Response of Karlsruhe Sand with calibrated parameters.

4. DYNAMIC ANALYSIS

In general, liquefaction occurs in saturated or nearly saturated sands subjected to cyclic loading (e.g. earthquake) and is characterized by a decrease in effective stress towards zero with a simultaneous increase in pore water pressure and a decrease in shear strength of shear stiffness under undrained conditions.

Cyclic mobility is a typical liquefaction fenomena which occurs in medium dense to dense sands, and it is characterized by progressive reduction in effective stress until reaching initial liquefaction. Buildup of pore water pressure results from alternate cycles of dilation upon shearing, and contraction upon stress reversal. Reduction in effective stress is gradual, and liquefaction occurs at a relatively larger number of cycles for denser samples. After onset of liquefaction there is a progressive accumulation of limited shear deformation in the process of repeating loss and gain of strength and stiffness [7]. In the post-liquefaction stage, sands experience a state change cycles, from solid-like to 'fluid-like' state under nearly zero effective stress [9].

The behavior of sands under undrained cyclic loading is affected by inherent factors (such as grain size, size distribution, shape, surface roughness) [14] initial conditions (e.g. density, fabric, effective mean pressure, stress ratio) and the load characteristics (e.g. amplitude of the cycles, cyclic stress ratio (CSR), application of stress or strain cycles) [15].

DEM has been shown to be able to capture the cyclic liquefaction behavior of sands. The constant volume method, assuming the particles and pore fluid to be incompressible, has been widely used by many researchers to simulate the undrained behavior of granular soils with the DEM due to been computationally straightforward.

In order to explore the fundamental mechanisms underlying the liquefaction phenomenon, DEM simulations become a key as they provide both macro stress-strain responses and particle-scale information. In this sense, several studies were carried out in the last decades and it was discovered that some void based fabric indices had a good correlation with cyclic stress-strain behavior on a macro-scale.

Ng and Dobry [16] first captured the cyclic liquefaction phenomenon in granular soils by means of the DEM. More recently, Wei et al. [9] studied microstructure and fabric evolution during pre and post liquefaction stages, proposed two particle-void based fabric descriptors to quantify void distribution's anisotropy and identified a unique hardening state line that defines the limit between the flow state and the hardening state, termed as the 'jamming transition'.

Wang and Wei [11] suggested the 'centroid distance', which is the difference between the particle mass center and the Voronoi cell mass center (used to divide the void space around each particle) to reflect the distribution of the void space surrounding the particles. This parameter presented interesting relations to the post-liquefaction shear strain generation and later saturation in 2D simulations.

Rui Wang et al. [10] introduced a new measurement called the 'Mean Neighboring Particle Distance (MNPD)' to reflect the amount of rearrangement needed for a granular assembly at liquefaction to reach a stable load-bearing state. This new fabric index showed the best correlation with post liquefaction shear strain development observed during undrained cyclic tests on sand.

Huang et al. [8] explores the evolution of mechanical stability and reversibility of the force transmission network during the cyclic liquefaction process through 3D simulations. They concluded that both flow liquefaction and cyclic mobility are related to the progressive degradation of the major force transmission network during cyclic loading, which becomes mechanically unstable upon liquefaction.

Martin et al. [12] investigated the influence of parameters characterizing the granular assembly (inertial number, geometrical and mechanical coordination number, redundancy index) leading to liquefaction of gravel when subjected to cyclic straning.

Based on the theoretical framework presented above, this study intended to simulate sand samples subjected to cyclic loading, in order to qualitatively compare the granular assembly response with what researchers obtained.

It should be noted that in all these studies the granular assembly's behavior subjected to cyclic loading is only qualitatively represented since the real texture and shape of a certain sand grains were not taken into account.

4.1. 2D BIAXIAL TEST

This work documents undrained cyclic biaxial tests performed with stress and strain cycles on granular assemblies consisting of spherical particles. The samples consist of 100 particles enclosed by rigid boundaries. Since the test is conducted to represent qualitatively the stress and strain characteristic responses, a small sized sample is chosen to save simulation time.

During the sample preparation state, samples were isotropically compressed to a mean effective pressure of $p = 30kPa$.

After sample preparation, the loading is applied as shown in Fig. 5 ensuring constant enclosed area by the four walls. This is done controlling velocities of the four walls surrounding the specimen, simultaneously moving the walls in the vertical and horizontal axis in equal strain rate applied and opposite directions. The cycles with stress and strain amplitude were applied ($q_{amp} = 10\ kPa, \gamma_{amp} = 0.08$).The contact stiffness is set to $5e8\ Pa$ and contact friction angle of $30°$. The stress and strain cycles were applied with a strain rate of $0.001\ s^{-1}$ in all tests, sufficiently slow to guarantee pseudo-static states throughout the simulations.

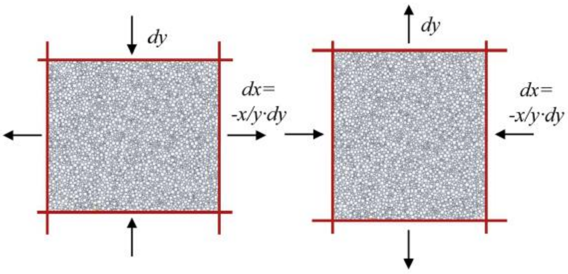


Fig. 5: Cyclic loading condition applied on the prepared sample.

4.1.1. Stress and strain path plot.

The results of cyclic biaxial tests by DEM simulations with strain and stress cycles are presented in Fig. 6.

The stress paths obtained resemble the "pore water pressure" buildup to initial liquefaction (in terms of progressive reduction of effective stress). In both cases a zero effective stress state ($p = q = 0$) was reached after a sufficiently number of cycles. Hysteresis loop formation and degradation, 'butterfly loop' shape of stress path after initial liquefaction are observed in Fig. 6 a), c).

Stress and strain paths can be differentiated between simulations with stress cycles and with strain cycles. In the first one, the amplitude of the cycles is given by the deviator stress 'q', so in the graph q vs. p, the shear stress remains within the given limits, while in the simulations with strain cycles the stress 'q' decreases as the effective pressure 'p' decreases.

Another difference can be noted in the γ vs. q graphs. Simulations with stress cycles are able to successfully reproduce the generation and eventual saturation of shear strain through the series of liquefaction states that the material experiences during cyclic loading after initial liquefaction. On the other hand, in the simulations with strain cycles, shear deformation remains within the limits while the stress q decreases with increasing number of loading cycles Fig. 6 b), d).

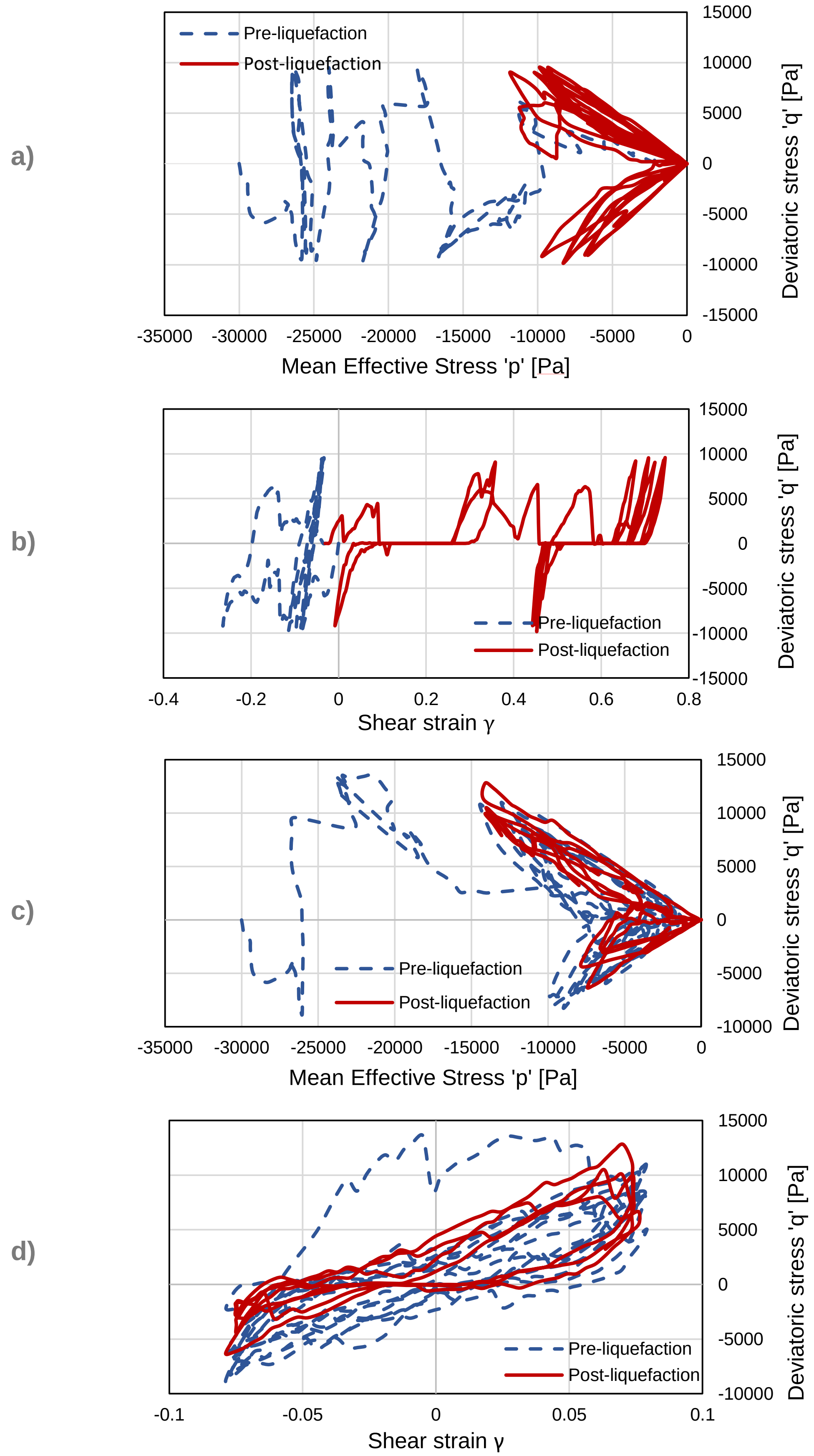


Fig. 6: Stress and Strain paths obtained from simulation for: a) and b) cyclic loading with stress cycles; c) and d) cyclic loading with strain cycles.

5. CONCLUSIONS

This research work illustrates the versatility of the Discrete Element Method in the simulation of several geotechnical tests, providing a better understanding the underlying mechanics behind the behavior of granular materials.

A simple linear elastic normal contact with linear rotational moment law is proposed to simulate the response of particles over up scaled grain size distribution of Karlsruhe Fine sand, numerical simulations of drained triaxial tests using DEM show good correlation with the experimental results, but there is still some difficulty to represent particles angularity only with contacts moments.

Cyclic tests were performed to obtain qualitatively the dynamic response of granular soils under cyclic loading with stress and strain cycles. Sand's liquefaction-to-post-liquefaction behaviors obtained in DEM simulations according to the counterpart observations in published work is shown, thereby validating the adopted simulation method for the proposed objective.

6. AKNOWLEDGEMENTS & PERSONAL ACQUIRED EXPERIENCE DURING THE RESEARCH STAY

First I would like to thank the Bavarian University Center for Latin America (BAYLAT) for this wonderful opportunity to carry out this exchange and being able to work at the Technical University of Munich as an exchange student. I want to express my gratitude to Prof. Andres Peña Olarte, Prof. Roberto Cudmani and Prof. Abel Jacinto for their guidance and motivation throughout the process. Finished this period, I can assure learning was continuous and deeply enriching in many aspects.

Regarding the academic experience acquired, I would like to highlight the pleasure of having attended for a short period of time the Center for Geotechnics at the TUM, equipped with the latest technology in installation of geotechnical testing equipment, and formed by a professional staff who perform with excellence in research work and multidisciplinary engineering consultancies. I had the opportunity to interact, work and learn from them, which gave my first research experience a high standard of professionalism, during which I felt accompanied and academically guided by the establishment members.

As for my personal experience, in general terms I would value it as pleasantly positive and fulfilling. In my case, doing the exchange by myself meant for me a valuable opportunity of self-discovery in which I could experience independence and autonomy when making decisions. I learned to fend for myself in a totally different environment than the one I was used to all my life. The culture shock of living in a European country, coming from Latin America, is enormous and I can assure I had continuous personal growth during those five months. I am also aware that being part of this type of experience provides great benefits for the professional future which I am training for.

Germany is an exceptional country, its landscapes, its people and its culture are 100% worth knowing. Despite the fact that my stay in Munich took place under extraordinary circumstances, due to the global COVID-19 pandemic, and even though being away from home and my family, I felt safe and free of dangers at all times. Fortunately I was able to squeeze the end of my stay in relative normality, allowing me to give closure to my research work and enjoy some summer activities. I also highlight the opportunity this experience was for making new friends both from Germany and multiple countries around the globe. This cultural exchange opened my mind to the recognition of a diverse world and I consider it truly priceless.

On the other hand, I would like to mention the experiences that were challenging for me, as I would not rate them as negative. The exchange itself, requires adaptation and total responsibility when staying abroad and carrying out the planned academic tasks, in order to develop professional and human skills. Furthermore, even though I have basic knowledge of the language, I feel that it would have been more profitable if I had a higher German level, since sometimes communicating was difficult for me, but still people in a greater percentage are trained and willing to communicate in English as an international language. I also think it is important to comment from my experience, that particularly in Munich, the cost of accommodation is high and there is a high rentals demand, so I would recommend students who have intention of making there the exchange, to try to find accommodation well in advance and provide themselves with the information needed to do it successfully.

To conclude, I would like to encourage students who could read this personal assessment to make this kind of academic exchange, and to dare to discover all that Bavaria has to offer. It is truly a life experience not to forget.

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