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Modeling of Triaxial Pressure Tests with Uniform Granular Materials Discrete Particle Method

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Abstract: Predicting the mechanical behavior of the soils on which the structures and facilities are built is crucial in civil engineering. Although solutions are made by modeling the soils as continuous homogeneous environments due to their ease and fast solutions, the soil is the combination of particles in a multiphase environment. Therefore, the Discrete Element Method, which offers a closer approach to the soil properties, was used in the study. This study modeled the behavior of homogeneous granular materials under triaxial compression tests using the Discrete Element Method (DEM). DEM, an ideal numerical technique for simulating particle environments, was used to investigate the mechanical responses of granular assemblies when subjected to varying confining pressures. The research focused on the effects of particle shape, size distribution, and contact mechanics on the material's stress-strain relationship and deformation behavior during the test. Using the DEM approach and PFC3D, the triaxial compression test of uniform sands was modeled to estimate the Poisson's ratio, Young's modulus, and bearing capacity.

Keywords: Discrete element method, PFC3d, triaxial pressure test

Öz: Yapı ve tesislerin üzerine inşa edildiği zeminlerin mekanik davranışların tam ve doğru olarak tahmin edilmesi inşaat mühendisliği açısından çok önemlidir. Günümüzde gerek kolaylığı gerekse hızlı çözümler sunduğu için zeminler sürekli homojen ortamlar gibi modellenerek çözümler yapılsa da zemin parçacıkların çok fazlı ortamda birleşmesidir. Bu nedenle çalışmada zemin özelliğine daha yakın yaklaşım sunan Discrete Element Method kullanılmıştır. Bu çalışmada, üç eksenli basınç testleri altında homojen granüler malzemelerin davranışı Ayrık Eleman Yöntemi (DEM) kullanılarak modellenmiştir. Partikül ortamları simüle etmek için ideal bir sayısal teknik olan DEM, granüler düzeneklerin değişen sınırlayıcı basınçlara maruz kaldığında mekanik tepkilerini araştırmak için kullanılmıştır. Araştırma, parçacık şeklinin, boyut dağılımının ve temas mekaniğinin, test sırasında malzemenin gerilim-şekil değiştirme ilişkisi ve deformasyon davranışı üzerindeki etkilerine odaklanmıştır. DEM yaklaşımı ve PFC3D kullanılarak üniform kumların üç eksenli basınç testi modellenerek poisson oranı, young modülü ve taşıma kapasitesi tahmin edilmeye çalışılmıştır.

Anahtar Kelimeler: Ayrık eleman yöntemi, PFC3d, üç eksenli basınç testi

1. Introduction

Granular materials are commonly encountered in fields such as soil mechanics and civil engineering. These materials consist of individual particles in contact with each other, and their mechanical properties can vary greatly depending on the particles' size, shape, distribution, and interactions. Understanding the mechanical behavior of granular materials is critical to ensuring structural safety in geotechnical engineering [1]. However, due to the complex structure of such materials, classical continuum theories may not be sufficient to reflect the behavior of granular materials fully. Therefore, numerical modeling techniques such as the Discrete Element Method (DEM) have been developed to investigate the mechanical properties of granular materials in more detail [2].

DEM is a powerful method that simulates the interactions of particles forming granular materials by considering them separately. DEM was first developed by Cundall [1] to analyze rock mechanics problems and later applied to soils by Cundall and Strack [1, 3]. The analysis algorithm includes two stages. First, the interaction forces are calculated when the elements penetrate each other slightly. This force-displacement formulation is usually called the "Smooth contact" or the "Force-Displacement" method. As stated by Cundall and Hart [4], it really represents the relative deformation of the surface layers of the elements [4]. In the second stage, Newton's second law is used to determine the acceleration occurring in each particle, and new particle positions are found using these acceleration data integrated with time. This process is repeated until the fracture is achieved.

This method, developed by Cundall and Strack [1], is widely used to accurately model granular materials' deformation, fracture, and shear behavior [1, 5–10]. The micro-scale analysis capability provided by DEM allows for a detailed examination of particle displacements and interactions. This has made it possible to develop a deeper understanding of the mechanical behavior of granular materials.

In the discrete element method, other numerical methods include possible deformation between particles, i.e., one-sided contact. These methods are called "non-smooth contact" methods. There are two main classes of numerical integration for these methods: event-driven integrations, known as the "Event-Driven Method" (EDM) [11], and contact dynamics time integrations, known as the "Contact Dynamics Method" (CD) [12–15].

In the EDM method, when two solid particles touch each other, a collision (Event) occurs, and the velocity and angular velocities after the collision are determined by a collision operator [16, 17]. Since the method considers single-point contact, it transmits only one force, which is unsuitable for systems with many contact points (contacts) such as soil, rock, or concrete.

The CD method works with the integral of the contact forces as in EDM. Still, this method works on the non-accelerated movements and effects that are integral to the contact forces, not the forces themselves. Since DEM, EDM, or CD consider soil particles as non-deformable objects in time element numerical analyses, they offer limited performance when the deformation and stress of the components (particles) must be regarded as in a static framework.

A triaxial compression test is a laboratory test widely used to determine granular materials' shear strength and deformation properties. During the test, pressure is applied to the sample in three axes to examine the material's behavior under different pressure conditions [18, 19]. While traditional experimental methods reveal the general trends of these behaviors, DEM-based simulations contribute to a more accurate interpretation of the experimental results by examining the microscopic interactions between particles in more detail [20, 21].

DEM has been used in geomechanics in various fields in recent years, from soils to intact rocks. Its applications have spread to many fields, including rock engineering, soil mechanics, mining, and petroleum engineering. DEM codes are primarily used in two-dimensional studies such as disks, ellipses, and polygons [22], whereas today, with the help of three-dimensional DEM computer programs, analyses can be made by summing up particles such as balls, ellipsoids and even polytropes [4]. The DEM method is applied to study the behavior of cohesionless and granular materials. However, the lack of testing capabilities to determine particle model parameters at the particle scale is a significant limitation in using DEMs. Therefore, the selection of parameters is based on trial and error by approximating the simulation results to laboratory results.

This study discusses the DEM modeling of the triaxial compression test on uniform granular materials. First, the properties of uniform granular materials and the theoretical basis of DEM simulations are examined. Then, the modeling of triaxial compression tests is evaluated in light of previous studies in the literature. By modeling uniform sands with a diameter range of 0.075 to 1.0 mm with PFC 3d (Particle Flow Code in three dimensions, version 3.0), the effects of particle model parameters on the stress-strain curve, shear strength, and elastic modulus of the sample are investigated, and the bearing capacity is calculated [23]. The success of DEM in predicting the mechanical behavior of granular materials is discussed.

2. Material and Method

For numerical analysis, uniform sands with diameters between 0.075 and 1.0 mm were simulated by modeling with PFC 3d (Particle Flow Code in three dimensions, version 3.0). The sample generation procedure with PFC3d is formed in four main steps. For each contact, the material strength is selected from a Gaussian distribution specified by the mean value and standard deviation. In programming, the FISH language is used to generate the three-axis test code in the PFC3D environment [23].

Step 1: Particle production and initial compaction

At the beginning of this step, a cylinder sample consisting of arbitrarily placed particles confined by three walls (top, bottom plates, and side cylinder wall) is produced by an expansion compaction method. To prevent particles from penetrating the walls, the average hardness of the walls is set equal to β times the average particle's typical hardness. The size distribution of the particles conforms to a uniform distribution characterized by the minimum and maximum particle radii. The porosity is set to 0.22 to calculate the number of particles that can be produced in the initially specified region.

Step 2: Loading the Specimen with the Specified Isotropic Stress

This step aims to reduce the magnitude of the locked-in stress that will develop after bonding (STEP 4). The magnitude of the locked-in contact forces caused by the particle deformation in STEP 1 will be close to the compressive forces during bonding. The isotropic stress, defined as the average of the three direct stresses in the main direction, is obtained by changing the radii of all particles equally at that time. To reduce the effect of the locked-in stress, the specified isotropic stress is typically set to a relatively low value against the material strength. The isotropic stress present in the assembly is calculated using the FISH code.

Step 3: Reducing the number of floating particles

Due to the characteristics where the irregular radius particles are randomly placed and mechanically compressed, fewer than three floating particle contacts may be present. All floating particles should be eliminated in the following surface placement stages to create a more realistic and dense bonding contact.

Step 4: Bond installation

Particles are allowed to stick together at the contacts to simulate material fusion. There are two bonding models in PFC3D. The contact bond model can be envisioned as two particles bonded over a small area at the point of contact only. The parallel bond model can be viewed as a finite-size plate-shaped contact acting on a circular cross-section extending in the plane of contact. Only forces can be transmitted through a force contact model.

A force and a moment can be transferred from the parallel bond model. While a particle cannot be attached to a wall, only particles can be connected. The bonds between particles are never renewed after they are broken. Parallel bonds are placed on all particles in physical contact throughout the sample, and then the μ friction coefficient of all particles is determined. The study created parallel bonds between the modeled particles, and their behaviors were investigated. The main material parameters used in PFC3d are shown in Table 1, and the particle model parameters are shown in Table 2. The model created using PFC3d is shown in Figure 1.

Table 1. Material properties used in PFC3d

Property	**Value**	**Symbol and Unit**
Density	1500	ρ, kg/m^3
Ultimate soil porosity	0,30	n
Parallel Bond Axial Stress	$1x10^7$	pb_nstren, N/m^2
Parallel Bond Shear Stress	$1x10^7$	pb_sstren, N/m^2

Table 2. Mineralogical properties of the RHA

Symbol	**Analysis 1**	**Analysis 2**	**Analysis 3**	**Analysis 4**
$k_n = k_s$ *(N/m)*	$1x10^8$	$5x10^8$	$10x10^8$	$15x10^8$
k_n / k_s	1	3	6	10
F_s (ratio)	0.5	1.0	2.0	3.0
pb_kn = pb_ks (N/m)	$6x10^9$	$8x10^9$	$10 x10^9$	$12 x10^9$

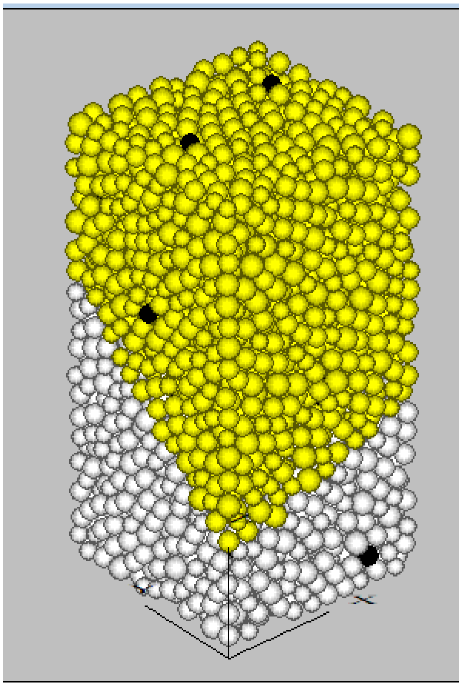

Figure 2. The model created using PFC3d.

3. Result

The elastic properties of the specimen can be determined by performing a loading/unloading test under elastic conditions (high bond strength and friction). Since the confining stress is constant (σ_d=σ_a), the test measured the initial Young's modulus and Poisson's ratio. The elastic properties of the specimen can be determined by performing a loading/unloading test under elastic conditions (high bond strength and friction). Since the confining stress is constant (σ_d=σ_a), the test measured the initial Young's modulus and Poisson's ratio. Equations 1 and 2 calculated the modulus of elasticity and Poisson's ratio as 230.08 MPa and 0.096, respectively.

$$E = \frac{\Delta\sigma_a}{\Delta\varepsilon_a} = \frac{\Delta\sigma_d}{\Delta\varepsilon_a} = \frac{1.349*10^6}{5.846*10^{-3}} = 230.8MPa \quad (1)$$

$$\upsilon = \frac{\frac{1}{2}(\Delta\varepsilon_x+\Delta\varepsilon_y)}{\Delta\varepsilon_a} = \frac{1}{2}\left(\mathbf{1} - \frac{\Delta\varepsilon_v}{\Delta\varepsilon_a}\right) = \frac{1}{2}\left(\mathbf{1} - \frac{\mathbf{4.694*10^{-3}}}{\mathbf{5.846*10^{-3}}}\right) = \mathbf{0.096} \quad (2)$$

For the sample model without contact bond, axial stress and axial deformation analysis against confining stress were performed and presented graphically in Figure 3. The analyses kept the density at 1500 kg/m^3, porosity at 0.3, friction angle 0.5 and particle diameters at 0.075-10 mm. The effect of particle axial hardness on soil behavior was investigated and analyzed.

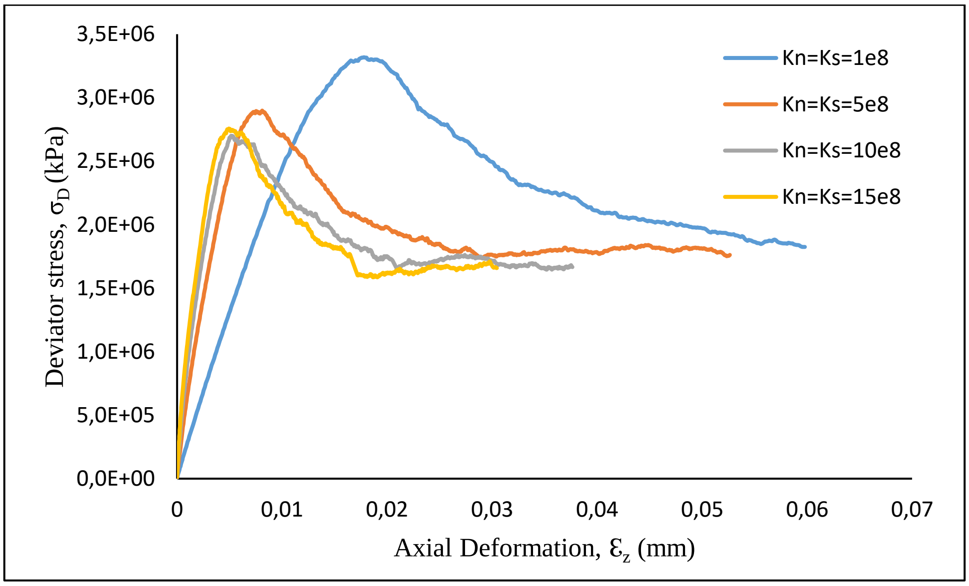

Figure 3. Analysis of axial deformation versus deviator stress for the sample model without contact bond.

In the analyses where the effect of the ratio of particle axial hardness to shear hardness of the parallel bonded model was investigated, particle axial hardness was used as 10e8 N/m, internal friction angle as 0.5, parallel bond axial hardness as 8e9 N/m^3 (pb_kn), parallel bond shear hardness as 1e9 N/m^2 (pb_ks), parallel bond axial tensile strength as 1e7 N/m^2 (pb_nstren), parallel bond shear tensile strength as 1e7 N/m^2 (pb_sstren).

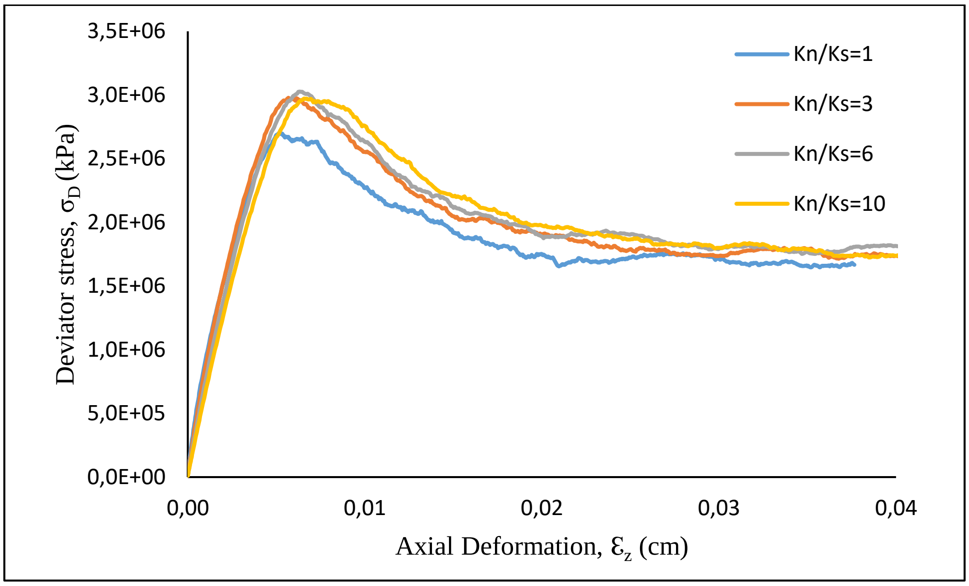

Figure 4. Effect of the ratio of particle axial hardness to shear hardness

In the analyses where the effect of the particle friction coefficient of the parallel-bonded model was examined, particle axial hardness 10e8 N/m (kn=ks), parallel bond axial hardness 8e9N/m^3 (pb_kn), parallel bond shear hardness 1e9N/m^2 (pb_ks), parallel bond axial tensile strength 1e7N/m^2 (pb_nstren), parallel bond shear tensile strength 1e7 N/m^2 (pb_sstren) were used.

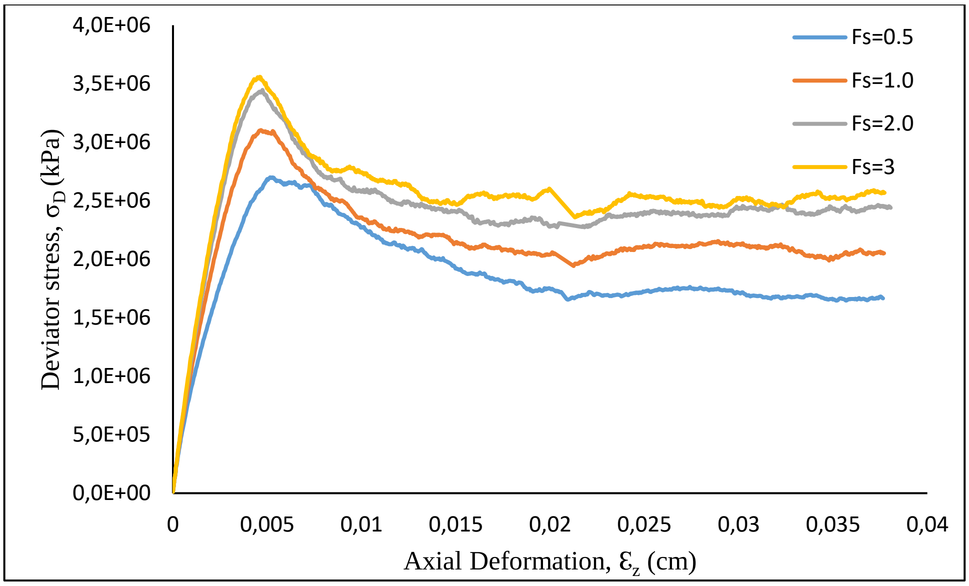

Figure 5. Effect of friction coefficient

In the analyses where the effect of parallel bond stiffness of the parallel bonded model was examined, particle axial stiffness 10e8 N/m (kn=ks), friction angle 0.5, parallel bond axial tensile strength 1e7N/m2 (pb_nstren), parallel bond shear tensile strength 1e7 N/m2 (pb_sstren) values were used.

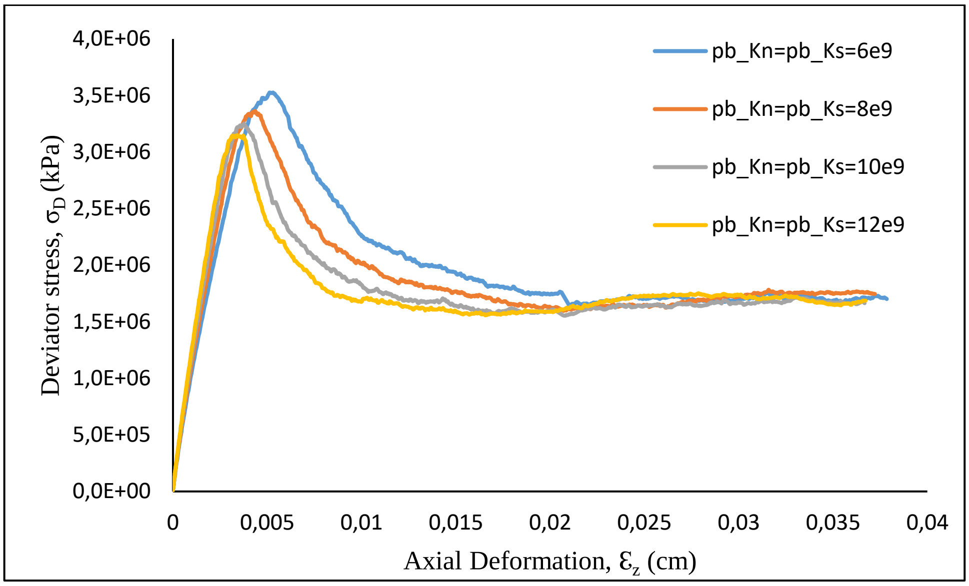

Figure 6. Effect of parallel bond stiffness

4. Discussion and Conclusion

As it is known, in this century the most important problems on a global scale are global climate change [24], pollution [25] and urbanization [26-28] is expressed. One of these problems is urbanization, which has increased rapidly in the last century, It is a problem that requires more people to live per unit area. To make it possible for more people to live per unit area in urban areas, is possible with the construction of high-rise and durable buildings, the foundation of which is building block is concrete [29-32]. Concrete is so widely used today that It is the most widely used building material after water and is an important part of building costs of the environmental pollution [33]. Therefore, in recent years, environmental pollution various waste materials as concrete admixtures. A large number of studies have been conducted on its usability. In these studies especially how admixtures affect the mechanical properties of concrete to determine the effects of the construction on the buildings and facilities [34-37]. In this study, it was also tried to be determined It is aimed to predict the mechanical behavior of the soils on which they are built. In order to provide an easier comparison of the analysis results, deviator stress and axial deformation results for different bond models are shown in Table 3.

Table 3. Deviator stress and axial deformation results obtained by analysis

Type of Bond Between Soil Particles	**Deviator Stress** kN/m^2	***Axial Deformation*** ***cm***
No contact bond	$1.672*10^6$	1.202
Particle contact bond bond strength: 0.05MN	$3.235*10^6$	1.170
Particle contact bond bond strength: 0.10MN	$5.833*10^6$	1.171
Parallel bond between particles	$3.630*10^6$	$7.572*10^{-1}$

In the laboratory, a sample with a diameter of 3.5 and a height of 7 cm was subjected to a triaxial compression test., The deviator load and axial deformation were measured at 3.15 MPa and 12 mm, respectively. The analysis showed that the contact bond condition is essential when uniform granular soils are modeled using the discrete element method. This method indicates that the parallel bond model gives close to actual results in modeling uniform sands.

In the study, the formation of peak stresses in analyzing triaxial compression tests is considered an essential point in understanding the mechanical behavior of granular materials. In particular, the effects of contact bonds and parallel bond models between particles on the peak stress are investigated.

When the parallel bond model was used, higher peak stresses were achieved because both force and moment transmission was provided between the particles. This model provided results that were particularly close to laboratory tests and allowed accurate prediction of peak stress values.

Since only the forces at the contact points were considered in the contact bond model, the peak stress values remained lower than in the parallel bond model. However, it was still helpful in providing information about the resistance capacity of the soil.

These differences were made more apparent by adjusting parameters such as soil particle hardness, friction angle, and bond strength. For example, the study showed that peak stress levels increased significantly by increasing axial stiffness and parallel bond axial tensile strength.

In this context, it was concluded that the peak stress values obtained accurately represent the bearing capacity and deformation properties of granular materials and provide critical data for the ground stability of structures.

Conflict of Interest

The author declares no conflict of interest.

Ethics Committee Approval

Ethics committee approval is not required.

Author Contribution

Writing-original draft, conceptualization, M.U.Y.

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