Studies and Analysis on Modeling Angular Soil Particles Using the Discrete Element Method

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Abstract: The Discrete Element Method was first introduced in 1979 to model granular soils within the context of geotechnical engineering. The material is modeled as a random assembly of discrete elements. Each particle interacts with neighboring particles through contact forces that can be built up and broken at any time. The particles were modeled as discs in 2-D or as spheres in 3-D. Research studies have been conducted to improve the simulation of actual grain shapes in (2003) developed the overlapping rigid clusters (ORC) method to accurately model irregular particle shapes. The idea relies on clumping a number of overlapping discs such that them coincides with that of the actual particle.

In this dissertation, experimental verification program is presented. An experimental setup was built and model-grains were manufactured in the laboratory. A numerical simulation for the experimental test was carried out. The numerical and experimental results were compared qualitatively and quantitatively. A good agreement was observed within small displacements ranges. However, results were considerably different at large displacements. Numerical results utilizing the ORC method were closer to the experimental results than those of discs. A sequential and operator-independent procedure, which relies on the ORC concept, was developed. Identical inertial properties between the actual particle and the model were ensured. The new procedure was implemented for rounded and angular particles.
The effect of particle shape and angularity on the strength and dilatancy characteristics of granular soils was investigated.

***Index Terms* - Discrete Method, Load Bearing Capacity, Environmental Engineering**

INTODUCTION- Modeling granular materials has been a challenging topic for decades. The particulate nature of granular materials controls their engineering behavior. The continuum assumption has been used to idealize soils and rocks, and numerical solution techniques such as finite element, finite difference, and boundary element methods have been successfully used to model these materials. The continuum mechanics models are phenomenological and are primarily concerned with the mathematical modeling of the observed phenomenon without giving detailed attention to the fundamental physical significance. The discrete nature makes the constitutive relationship complex and needs an excessive number of parameters to be able to model the behavior accurately. Another alternative is to model the granular materials experimentally using photo-elastic materials . This approach presented a physical basis for understanding the behavior of granular soils, but is experimental rather than numerical and is limited in terms of its ability to model real systems.

The discrete element method (DEM) offers an alternative approach to simulate the behavior of granular materials. The particulate nature is automatically simulated as particles are discrete and forces are transferred through the contacts between particles. The method can handle a wide range of materials constitutive behaviors, contact laws,

and arbitrary geometries. The Discrete Element Method (DEM) for modeling granular soils within the context of civil engineering was first introduced in (1979). The particles were modeled as a random assembly of discrete discs. Many research studies have since been conducted to improve the simulation of angular grain shapes.

LITERATURE SURVEY- Numerical modeling, supported with an accurate simulation of test conditions, soil parameters, constitutive models (FEM), and contact models (DEM), is a powerful tool to study physical phenomena. Numerical modeling provides the capability of performing extensive parametric studies because a large number of runs can be performed in a relatively short period of time. On the other hand, inaccuracies in determining soil parameters can affect the numerical modeling results dramatically. Experiments, however, reflect the actual behavior of the material provided that all the field conditions have been accurately simulated. The time consuming cost associated with building experimental setups are the main obstacles for the experimental work. Studying a certain phenomenon experimentally and confirming the results numerically may be the best approach and can reliably capture the response of the system with minimal cost.

DISCRETE ELEMENT METHOD FOR MODELING GRANULAR MEDIA-The particulate nature of the granular material usually governs the behavior of these materials. Pressure-dependent shear strength and stiffness, dilatancy, pressure history, and continuously non-linear stress-strain response are essential properties when studying the behavior of granular media.

The Discrete Element Method (DEM) for modeling granular soils was first introduced by Cundall and Strack (1979). The material is modeled as a random assembly of discrete elements, which is a better representation of the particulate nature of granular soils. Each particle interacts with neighboring particles through contact forces that can be built up and broken at any time. Different types of bonds can be applied between particles to simulate phenomena such as cementation. The particle assembly is governed by boundary and loading conditions. The DEM solves the dynamic equilibrium equations for each element subjected to either body or boundary forces. The method is capable of analyzing multiple interacting deformable continuous, discontinuous or fracturing bodies undergoing large displacements and rotations. In the scheme developed by Cundall and Strack (1979), the interaction between particles is monitored, contact by contact, and the instantaneous motion of the particles is computed accordingly. Deformation of the particles is not allowed. Instead, the particles are capable of "overlapping" at contact points as an alternative method to modeling individual particle deformation.

In DEM, the equilibrium contact forces and displacements are determined through a series of calculations tracing the movement of the individual particles. These movements are the results of the propagation, through the medium, of disturbances originating at the boundaries . The discrete element method, in the version proposed in (1979), is based on the idea that a small enough time step should be chosen to ensure that, during a single time step, disturbances do not propagate from any disc further than its immediate neighbors.

COUPLED DEM AND FEM-Coupled FEM and DEM simulations have been conducted such as that introduced in (1992). They introduced a method that can be used for modeling multiple interacting deformable bodies. The method was based on the assumption that deformation modes can be decoupled from rigid body motion. In this method, each deformable body was treated as an individual discrete unit, which was idealized by a finite element model. The discrete units may undergo large displacements and rotations. The interactions between these units occurred through contact forces that were continually updated.

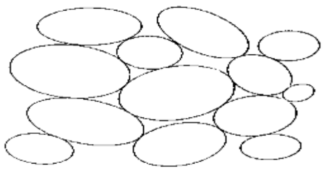
EXPERIMENTAL VERIFICATION OF DEM-Experimental verification of the ability of the DEM to capture the behavior of the granular soils has been of interest for many years in (1997) presented an automated video tracking and digital image analysis system that was developed to obtain soil particle displacement fields and velocities from small-scale laboratory experiments. A three-dimensional simulation of a laboratory plowing experiment was performed in which a one-to-one correspondence was achieved between the number of particles and their size distribution in simulation and physical experiment. The video tracking data were used to evaluate the numerical simulation in modeling the experiment kinematics. Good agreement was found between the experimental and the simulated deformation patterns.

In (2001) presented a comparison between a granular material studied experimentally in simple shear and numerical modeling using DEM. Simple shear tests were conducted inside the magnetic core of magnetic resonance imaging (MRI) equipment. Spherical pharmaceutical pills of were used as the granular material. The center of each pill was determined by the MRI. An experimental study was performed to determine the pharmaceutical pills properties required for the numerical modeling. Good agreement was found at both levels. Excellent agreement was found up to 10% shear strain. Beyond that, the peak shear points in the numerical results were slightly lower than those in the experimental results.

MODELING NON CIRCULAR PARTICLES-In the DEM scheme proposed in (1979), the granular particles were modeled as discs in 2-D simulations and as spheres in 3-D simulations (fig. 2-1). The resistance to rotation is much less for circular particles compared to that of the actual particles. Circular particles have an inherent tendency to roll. The macroscopic angle of shearing resistance for circular particles modeled using DEM is much less than that of the actual irregular particle assembly. However, the contact detection for the circular particles does not need complicated algorithms, and also the direction of the contact normal force is always toward the center. As such, the computed normal contact forces never contribute to the moment acting on a particle as each normal contact force always acts in the direction of the particle centroid. Different particle shapes rather than discs/spheres were proposed, in many research studies, to be used in DEM simulations in order to improve the numerical simulation.

Polygon particles were presented in (1992) and in (2000). Figure (2-2) shows a sample of polygon-shaped particles. A more realistic representation of the particle behavior can be achieved using polygon-shaped particles; however the method is computationally intensive.

A research realized that ellipse-shaped particles have fewer tendencies to rotate and also have a unique outward normal. They developed a numerical algorithm for the DEM using two-dimensional ellipse-shaped particles (fig. 2-3). A robust algorithm for computing particle-to-particle and particle-to-wall contacts was derived. The results of the validation tests indicated that the ellipse-based DEM resulted in mechanical behavior that was similar to that of real soils. Ellipse-shaped particles, however, do not accurately represent the particle shape. Ng (1994) developed a new program called ELLIPSE2. The new program was used to explain the stress-strain behavior of granular soils under monotonic drained compressive loading and cyclic constant volume loading at various shear strains. A 2-D random assembly of elastic rough quartz particles was used to simulate the granular soil particles. Good agreement was observed between the numerical and the experimental results. The results confirmed that DEM simulations using an assembly of circular and elliptical particles give a better representation of the behavior of granular soils. On the other side the influence of the contact of two-dimensional ellipse-based particle on their interaction. The samples were isotropically compressed and then sheared in biaxial compression. In order to assess the relative



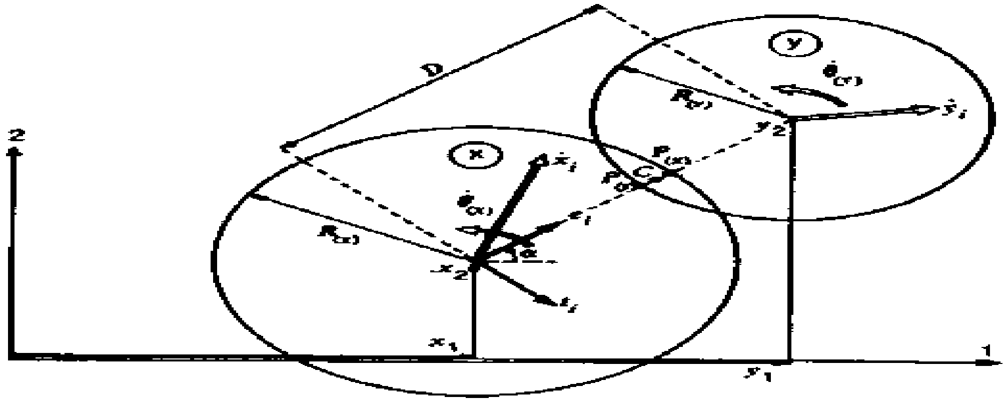


Figure 2-1. Two circular particles in contact

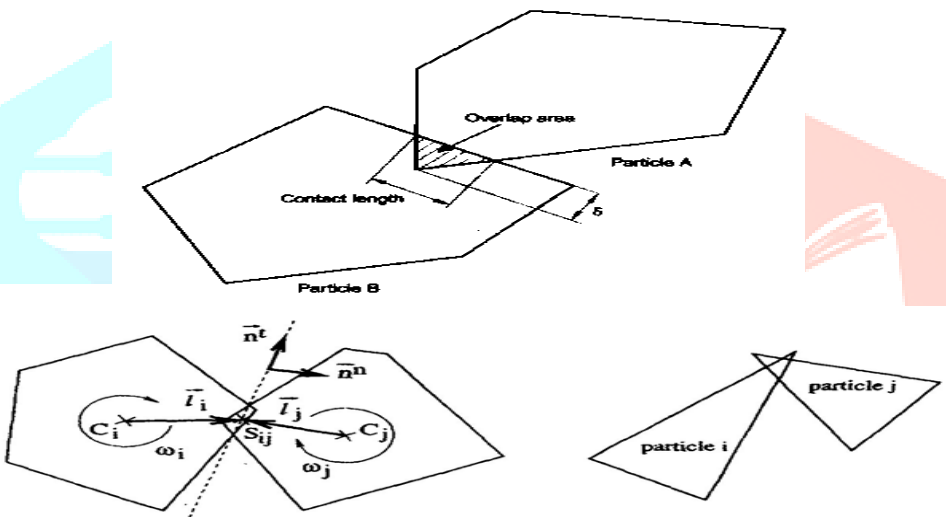
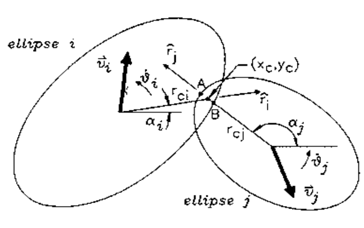


Figure 2-2. Polygon-shaped particles



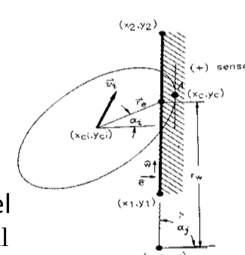


Figure 2-3. Ellipse-shaped particles: particle assembly, two el
contact between an ellipse-shaped particle and a wall

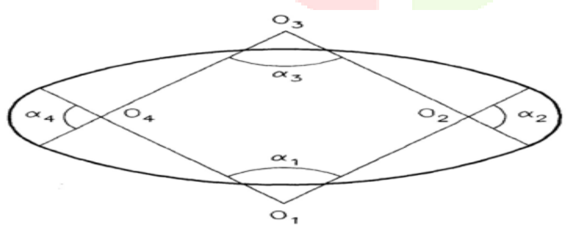
importance of rolling and sliding, the contact deformation were separated into portions:

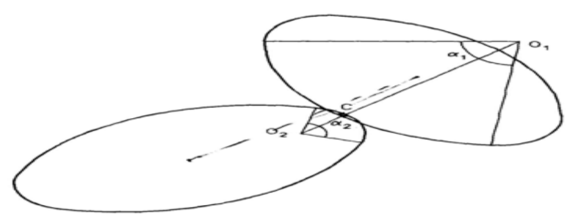
due to individual particle rotation, and (ii) due to particle translation. This decomposition demonstrated that particle rotation accounts for twice as much contact motion for round particles as particle translation. rotation were observed with the ellipsoid assembly during the triaxial test. The results demonstrated that using non-spherical particles in discrete element modeling is essential to improve the simulations of granular materials.

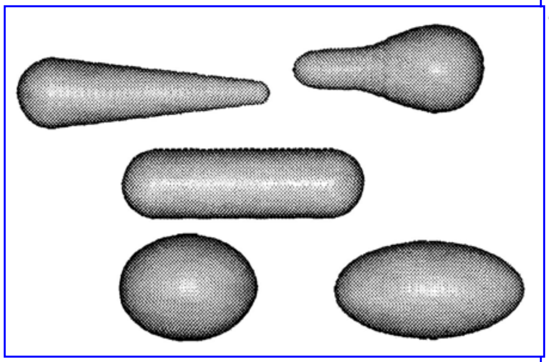
Another research proposed a computationally efficient model for the discrete element.

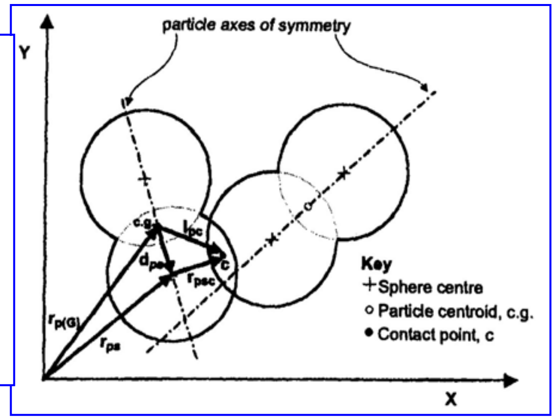
simulation of non-round particles. The idea is to approximate the ellipse by an oval shape whose boundary is determined by four circular arches of two different radii that are joined together in a continuous way (fig. 2-4). More complex shapes can be reproduced by changing the radii of the arches. The idea is computationally efficient because the determination of the contact and overlap between two circular arch segments is very similar to that of circles in the original DEM code. The application of the idea in 3-D was not presented. A direct test of the method's performance indicated that it is very effective and less than two times slower than the corresponding circular models.

In (1999) presented a method to model axisymmetrical particles as multi-sphere discrete elements. The particles are re-generated using overlapping spheres with fixed rigidity with respect to local coordinate system (fig. 2-5). The method can theoretically model any shape, however highly angular particles cannot re-generated properly. Favier et al. (2001) used the proposed method to model the discharge of ellipse-shaped particles through an orifice in a flat bottom hopper. The simulations were compared to the experimental results at the same scale. A good agreement was noticed between the flow behavior pf the simulated and physical particle assemblies for all orifice sizes.









FUTURE SCOPE-The critical state lines corresponding to circular particles using different interparticle friction coefficients are shown in fig. (5-54). The critical state lines shifted up and became more steep with the increase of the interparticle friction coefficient. Contraction was observed for (f = 0.25) under confining pressures of 250KPa and 500KPa because the initial conditions define a contractive soil. The results show that the numerical simulations are very sensitive to the selected interparticle friction coefficient/angle.

As stated in many research studies, the main obstacle to the DEM is that simulations are time consuming especially when actual particle shapes are used along with large number of particles. Unless the DEM is able to simulate millions of particles with their actual shapes, no actual scale problems can be accurately simulated. Another alternative is to change some properties of circular particles to control their behavior such

that they reproduce the behavior of angular particles. The circular particles, although not a true representation of the particles, are the most efficient shape to model. Computation time is very small compared to the most effective alternative schemes that utilize other shapes.

Interparticle friction coefficient is one of the most significant properties in DEM simulations. As shown in fig. (5-54), the interparticle friction angle affects the position of the critical state line. It was observed also that the critical state lines for different angularity and shape groups were shifted up with respect to that of circular particles. To this extent, it may be possible to adjust the interparticle friction angle to account for the particle shape characteristics. The target interparticle friction coefficient can be extracted by re-plotting the critical state line for the required angularity or shape group on top of the critical state lines shown in fig and choose the interparticle friction that matches the critical state line for the group.

CONCLUSION-An experimental setup was built and model particles were manufactured and modeled numerically. The experimental test results of five identical tests were compared qualitatively and quantitatively with the corresponding numerical simulation. The ORC technique was found to be effective in modeling the behavior of angular particle assemblies. While particle displacements and rotations of both the numerical and experimental systems were almost identical at small displacements, larger differences were observed at high displacements, even among the five experimental tests that have been performed ensuring identical initial and boundary conditions. This variability is

attributed to minor changes in the initial conditions, as well as other inherent uncertainties in the system, and cannot be avoided. The ORC simulated system behavior is within the range of the five experimental tests. The experimental validation was extended to a different type of sands. The experimental setup was altered to induce a different mode of disturbance to the model grains. A parametric study has been conducted to study the effect of interparticle friction, contact stiffness, and global damping on the rotations and displacements of the model particles. The results indicated that the global damping is a critical parameter in DEM modeling and must be carefully selected. The effect of interparticle friction and normal contact stiffness on the response was also evaluated.

A modification for the ORC technique was presented and verified for both rounded and angular particles. The modification ensures an identical mass, center of gravity, and mass moment of inertia for both the actual and the created particles. A conditional element addition sequence was proposed in order to facilitate the future automation of the procedure. The compatibility equations were imposed to the compatibility elements/discs to determine their modified density. The method was verified manually using Gomti river sand particle # 4 as a highly angular particle and Ghaghra sand particle # 1 as a rounded particle. The modified ORC method was found to be applicable for both sand particles and should be applicable for almost all particle shapes, which may need more iteration to reach the final densities. The modified ORC can be considered a step forward in improving the modeling of angular particle using DEM especially in dynamic applications.

Discrete element numerical simulations of pure shear conditions were performed for different particle shape and angularity groups. The modified shape factor and the angularity factor were used to separate particles into shape and angularity groups. The stress-strain-volume curves were presented and analyzed. The critical state lines for shape and angularity groups along with the corresponding lines for circular particles were determined. The critical state lines, for different shape and angularity groups, were shifted up compared with that of the circular particles, which indicates an increase of volumetric strain and hence dilation. The effect of interparticle friction coefficient on the behavior was studied.

Again, the critical state lines showed significant dependency on interparticle frictions. An attempt was made to use an equivalent interparticle friction to model different particle shapes. It was concluded that there is no one-to-one equivalency between interparticle friction and shape or angularity. Instead, the interparticle friction must be continuously altered as a function of confining pressure and void ratio to achieve the required effect.

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