Three-dimensional Interaction of Granular Media Simulated by Discrete Element Method

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Abstract

Despite of being a vigorous constituent of natural and built environment, three dimensional interaction and behavior of the granular media is not yet convincingly understood. As a part of the progressive effort to achieve this goal, a three dimensional numerical model , based in Discrete Element Method (DEM), is developed and validated for fundamental principal of energy conservation and elasto-plasticity of the material. The model successfully simulates the conservation of total energy, pure elastic and elasto-plastic behavior of granular material. A plain strain compression test is also performed on the three dimensional specimen of the material, with- and with-out the pre-consolidation pressure to reproduce field conditions. A typical behavior of stress ratio with a peak value followed by strain softening has been successfully replicated. The void ratio has shown a trend of first decreasing and then dilating before becoming constant, which is in close agreement to the actual behavior.

Keywords: Numerical modelling,discrete element method, granular media, validation, visco-elasticity, plain strain compression

1. Introduction

Abundance of granular media makes it more attractive for many professions (civil engineering, chemical engineering, production engineering, powder technologies etc.), however its complex interacting behavior is not yet fully understood, e.g.; it deforms like solids (Peters and Dziugys 2002), flows like liquids and compresses like gases. Physical modeling and subsequent micromechanical studies of such a media was practically less fruitful, though some efforts have been made to understand/compute the stress-strain response of soil using photo-elastic experiments (Oda, Nemat-Nasser, and Konichi 1985). Many researchers are concentrating their efforts on numerical modeling in their recent endeavors to understand well the failure mood and micromechanics of granular media. Phenomenal advancements in computing technology in recent years have enabled the researchers to simulate the granular media to study its interactive behavior and subsequent failure mechanisms under different boundary conditions (Cleary 2004).

Discrete nature of granular media primarily requires a discontinuous simulation method; therefore, Discrete Element Method (DEM) is unanimously considered the best approach to deal with the granular media studies (Kozicki and Dons 2008). This method allows covering a wide spectrum of phenomena like laboratory and field tests, landslides and slope stability issues, shallow and deep foundations, macro and micro level failure responses, seepage and permeability problems (Catherine 2011). DEM uses a fundamental and basic philosophy of considering each particle as an element, which explicitly withstands stresses and strains. These elements interact solely at contacts and observe Newton's laws of motion, under the actions of external forces like force of gravity, axial stresses etc. The material response (macro and micro level) is then determined using individual movement and mutual interaction of huge population of elements.

In this work, a three dimensional numerical model is developed to simulate granular interaction and several tests are carried out to ensure its practical validity.

2. An overview of Discrete Element Model

With an enormous development in the field of computing power and numerical algorithms, there could be multiple options for the solution to problems of increasing complexity. However, discrete element method (DEM), owing to its distinctive features, has been regarded as most efficient and effective method to deal with granular media. DEM was first introduced by Cundall (1971) to address the problems of rock mechanics. Since then, significant progress has been made in the development of DEM methodologies and applications. In DEM, the basic particles are considered to be rigid (i.e.; they possess a finite mass and rotational inertia) and each particle is independent to have translation and/or rotational movement. The contact between particles occurs over an infinitesimal area and each contact involves only two particles. The equilibrium contact forces and displacements are determined through a series of calculations by tracing the movement of the individual particles. The time step for these iterations should be small enough that the disturbance of any particle cannot propagate farther than its immediate neighbour (Starck and Cundall 1979; Lunding 2008; Cundall 1988a; Thornton 2000; and Rowe 1962).

In this study, a numerical model, rooted in discrete element method, is developed to simulate three dimensional interactions of spherical shaped granular particles. This model is actually the extension of a two dimensional model, developed by Iwashita and Oda (1998) and used in many of his works like; the study of rolling resistance at contacts in simulation of shear bank development (Iwashita and Oda 1998), the study of micro-deformation mechanism of shear banding (Iwashita and Oda, 2000), the study on influence of inherent anisotropy on micromechanical behaviour of granular materials (Mahmood and Iwashita 2009), the study of microstructure evolution inside the shear band in biaxial compression test (Mahmood and Iwashita 2011). The contact mechanism is modelled by a hard sphere-soft contact model, in which an overlapping is allowed at all contact points (as shown in Fig. 1).

This overlapping distance $u_n u_n$ (normal to contacting particles) for two spheres A and B with their radii as r_a r_a and $r_b r_b$, respectively, can be calculated by Eq. (1)

$$u_n = \sqrt{\{(x_b - x_a)^2 + (y_b - y_a)^2\}} - (r_a + r_b)$$

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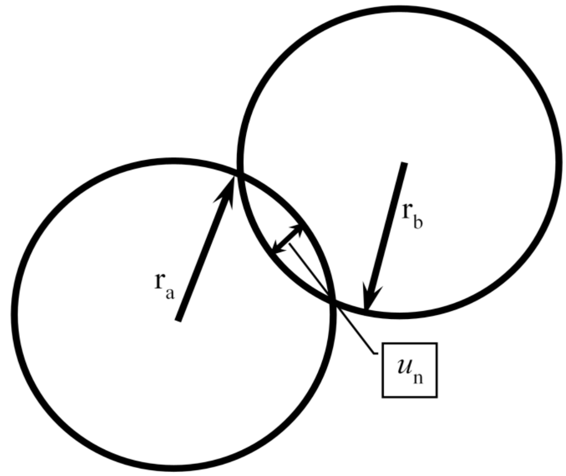

Fig. 1: Contact mechanism and overlapping between two spherical particles

Normal force at contact point is then determined by Eq. (2) using the overlapping distance:

$$f_n = \begin{cases} k_n u_n + C_n \frac{du_n}{dt} & u_n < 0 \\ 0 & u_n \geq 0 \end{cases}$$

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where k_n k_n and $C_n C_n$ are spring coefficient and damping coefficient in normal direction, respectively. And u_n is the deformation or overlapping along the centre lines of the two contacting spheres.

Similarly, tangential force can also be calculated by Eq. (3);

$$fs = \begin{cases} k_s u_s + C_s \frac{du_s}{dt} & abs(k_s u_s) < k_{lim} u_n \\ sin(k_s u_s) \times k_{lim} u_n & abs(k_s u_s) \geq k_{lim} u_n \end{cases} \quad (3)$$

where k_s, C_s, k_{lim} and u_s k_s, C_s, k_{lim} and u_s are tangential spring coefficient, tangential damping coefficient, limiting value of spring coefficient and tangential overlapping distance, respectively, whereas 'abs' represents the absolute value.

Linear Kalvin model is employed to simulate normal displacement, whereas a shear slider with shear stiffness (k_c) is used to capture the sliding resistance (as shown in Fig. 2a). This shear slider becomes functional when normal forces (f_n or N) and tangential forces (f_s or μN) at any contact point hold the following inequality:

$$| f_s | \geq \mu f_n | f_s | \geq \mu f_n \quad (4)$$

where, μμ is the coefficient of friction between two particles.

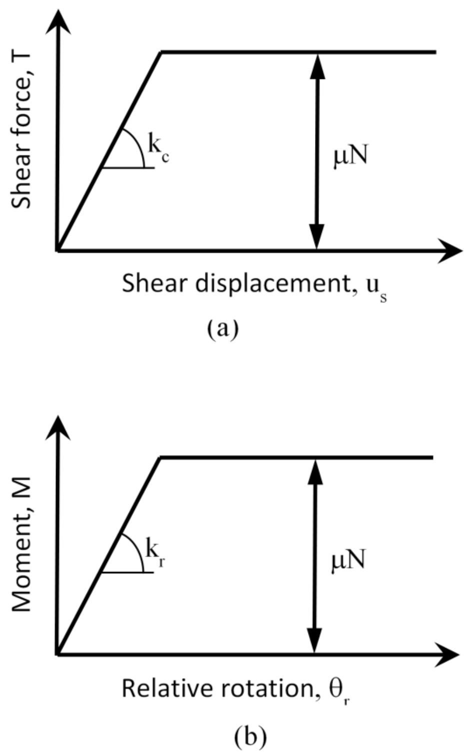

Fig. 2: Sliding and rolling at a contact: (a) Sliding; (b) Rolling (after Iwashita and Oda 1998)

In order to simulate the shear band (micromechanical behaviour) of granular media (Abdalsalam and Gutierrez 2010; Pengcheng and Yannis 2012), rolling resistance is measured through a set of spring, dash pot, no-tension joint and a slider as shown in Fig. 3. Rolling resistance moment is calculated using Eq. (5).

$$M = -k_r\theta_r - C_r\frac{d\theta_r}{dt}M = -k_r\theta_r - C_r\frac{d\theta_r}{dt} \quad (5)$$

where, k_r and C_r are rolling stiffness and viscosity coefficient, respectively. Slider for rolling become functional provided moment M crosses a limiting value of ηf_s (Fig. 2b)

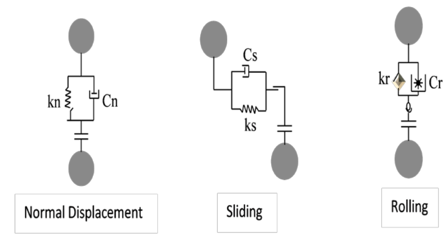

Fig. 3: Contact model using springs, dashpots, sliders and no-tension joints (after Iwashita and Oda 1998)

$$|M| \geq \alpha f_n |M| \geq \alpha f_n \quad (6)$$

where, α is the coefficient of rolling friction.

3. Validation and Calibration of Discrete Element Model

Any numerical model needs to be validated analytically and experimentally before using it for complex geotechnical problems, as proposed by (O'Sullivan, Bray, and Cui 2006) and many others. Most convenient and practical approach is to first simulate some small scale and simplified phenomenon before leading to complex and real problems. Calibration of results against experimental data and/or field measurements is required in any case. For the subject study, validation of numerical model is first checked by using some small scale and simplified tests for energy conservation and dynamic relaxation. Furthermore, two biaxial compression tests are performed on relatively complex models to study the qualitative response of spherical shaped particles.

3.1 Energy conservation test

To verify the dynamic stability of the numerical model, a stack of nine (09) spherical balls, discrete in nature, is used to check conservation of total energy in the system. The first ball is placed on a rigid wall (fixed in space) and the remaining balls are stacked on the top of each other such that there is no initial contact force at any of the contact, as shown in Fig. 4.

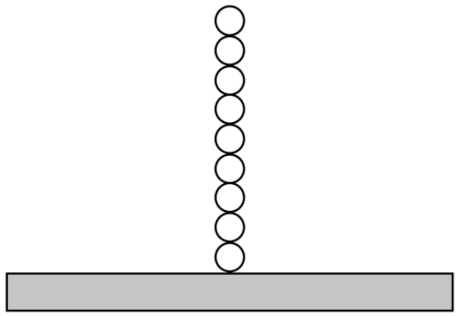

Fig. 4: Stack of nine balls and their initial position to study energy conservation of the system

The diameter of each ball is 1.0 m and density of the material is 2600 kg/m^3, which makes mass of each ball equal to 1,361 kg and the gravitational acceleration as 9.81 m/s^2. The top surface of the rigid wall is considered as datum for this test and its coordinates are set as (0,0,0). The total energy of the stack at the beginning of the test is only gravitational energy, which equals 540.73 kN-m. Moreover, it was ensured that there is neither any gain nor any loss of energy in terms of mechanical energy, damping or friction etc.

3.2 Elasticity and visco-elasticity test

For simplicity, soil is modelled as elastic material in some cases. However, its actual behaviour is more close to that of visco-elastic material. To make sure that proposed numerical model successfully envisages actual soil behaviour, the same balls stack set up is used in a different way. Only one ball is taken from the stack and released from an elevation of 0.75 m with a clear height of 0.25 m (radius, R = 0.5 m) as shown in Fig. 5. The damping ratio for the ball is taken as 0.05 (5.0 %).

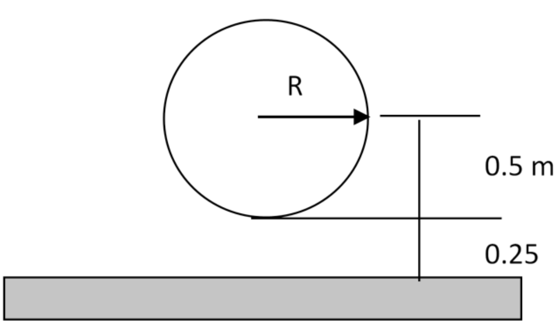

Fig. 5: Single ball setup at its initial position to investigate elasticity and normal dynamic relaxation of the model

3.3 Biaxial compressional test

A three dimensional specimen of spherical soil particles (as shown in Fig. 6), having dimensions of 1.5 x 1.5 x 3.0 and aspect ratio of 2.0, is used to perform a plain strain compression test with a prior uniform compression. The specimen is composed of 6,750 spherical particles with their diameters varying from 0.3 to 0.5 m with a constant value of 0.75 as friction coefficientcorresponding to 36.9 degrees of friction angle, representing a course grained granular material. Each particle is assigned a predefined position in a uniform and regular grid; however, its diameter is randomly selected by the program. The X-Z and Y-Z boundaries are considered flexible, to transmit confining pressure to the inner particles, while the top and bottom boundaries (in X-Y plane) are considered as rigid walls. Plain strain compression test is performed in two stages. First, a prior uniform compression is applied in which the specimen is allowed to compress under a specified confining pressure. In second stage, loading is applied to the specimen in the form of strain through top and bottom rigid walls, while maintaining the same confining pressure which is used for its prior compression.

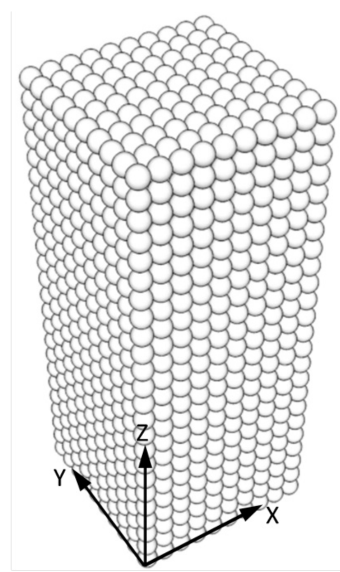

Fig. 6: Three dimensional arrangement of spherical particles to perform plain strain compression test

4. Results and Discussion

Detailed discussion about the results, for all the validation test setups described in section 3, is made in the following sub-sections

4.1 Energy conservation test

The total energy of each ball in the stack of nine (09) balls, shown in Fig. 4, consists of three components: kinetic energy, potential energy and gravitational energy. In this test, only gravitational force is applied to the stack of balls and the balls are released from their initial position. The balls are pushed into each other and continue to oscillate up and down forever, conserving the total energy as expected and shown in Fig. 7.

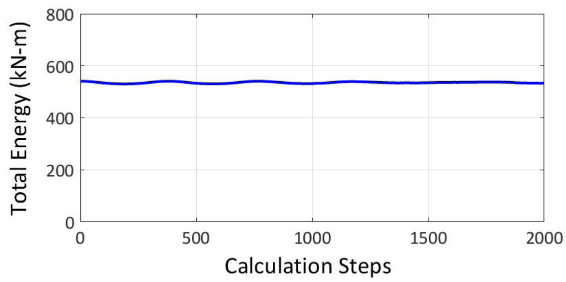

Fig. 7: Total energy of a stack of nine balls, shown in figure 4

4.2 Elasticity and visco-elasticity test

Elasticity and visco-elasticity are major parameters in the proposed numerical model for two reasons. First, the material in granular media which behaves visco-elastically; secondly, since DEM is originally designed to solve dynamic problems with explicit integration for static problems, dynamic relaxation (damping) must be performed in order to achieve convergence. Besides the afore mentioned two reasons, the magnitude of damping coefficient is very critical as excessively small value can lead to spurious vibrations, to which granular media are very sensitive. On the other hand, sufficiently large magnitude can result in simulation of the material as immersed body system, which is not the case in reality.Fig. 8 convincingly shows that elastic and visco-elastic behaviors of the system are precisely modelled.

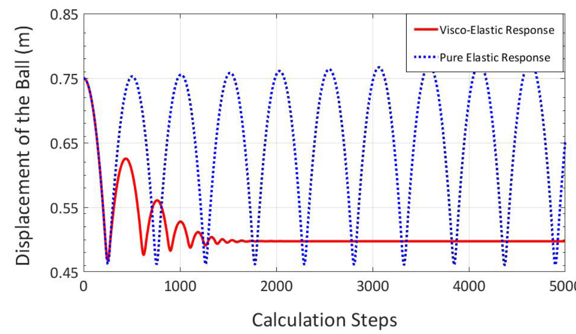

Fig. 8: Displacement versus time plot of the ball, shown in figure 5, both with- and with-out dynamic relaxation

The ball keeps on oscillating around its initial position when modelled without damping and released from an initial clear height of 0.25 m above a rigid wall surface. When the normal dynamic relaxation (damping ratio = 0.05 or 5.0 %) is applied, the vibration attenuates considerably over time and the ball takes practically a static position after fifteen hundred (1500) iterations, while touching the rigid wall surface.

4.3 Biaxial compressional test

4.3.1 Pre-consolidation and stress release

Soil samples extracted from the field to perform laboratory experiments are often disturbed; the degree of disturbance depends on the method of extraction and type of sampler though. One typical disturbance for samples taken for compression or consolidation tests is the loss of confining pressure from adjoining soil. Therefore, a pre-consolidation pressure is applied to reproduce field conditions before performing laboratory compression or consolidation tests. To simulate this phenomenon in the proposed numerical model, a pre-consolidation pressure is applied to the specimen shown in Fig. 6 by using a confining pressure of $1x10^5$ N/m^2. At this stage of the analysis, only top, bottom, right and left rigid boundary walls are used to transmit the confining pressure to the inner particles, while front and back walls remained inactive in the stress transfer.

Average velocity of all particles is plotted against calculation cycles in Fig. 9. The plot shows a drastic decrease in average velocity of particles as time passes. The particles are first displaced at a very high speed of 12 m/s because of their initial configuration at a regular grid. However, under the effect of hydrostatic confining pressure, they soon came in contact with the neighboring particles, which forced those to slow down to almost zero velocity in just 100,000 iterations.

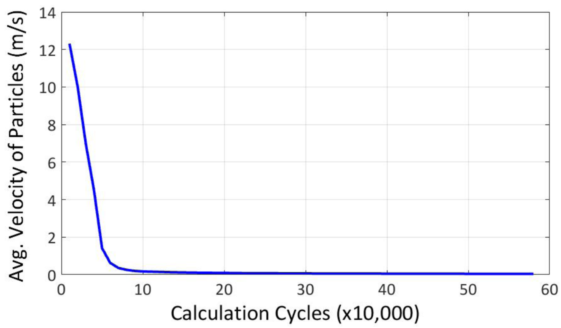

Fig. 9: Velocity profile of all particles of three dimensional sample (shown in Fig. 6) over time

4.3.2 Plain-strain compression test

Plain-strain compression test is performed on the three dimensional specimen of spherical particles, shown in Fig. 6, for both the conditions of with- and with-out pre-consolidation.

For the case of without pre-consolidation, the axial stress $(\sigma_{11})(\sigma_{11})$ is applied by moving top and bottom rigid wall boundaries while the lateral stress $(\sigma_{33})(\sigma_{33})$ is kept constant through flexible boundary. The axial strain is then calculated by Eq. (7);

$$\varepsilon_{11} = {}^{\Delta H}/_{H_o} \varepsilon_{11} = {}^{\Delta H}/_{H_o}$$
(7)

where, $H_0 H_0$ is the initial height of the specimen and $\Delta H \Delta H$ is change in the height of specimen.

For pre-consolidated case, the sample is first consolidated under a hydrostatic confining pressure of 1x10^5 N/m^2 using top, bottom, right and left rigid wall boundaries. In second stage, the right and left rigid wall boundaries are replaced with flexible boundaries and axial strain $(\varepsilon_{11})(\varepsilon_{11})$ is applied through top and bottom rigid wall boundaries.

Fig. 10 shows a plot of stress ratio $({}^{\sigma_1}/_{\sigma_3})({}^{\sigma_1}/_{\sigma_3})$ against axial strain which is well consistent with the stress strain pattern of granular media. The stress ratio first increases with axial strain until it reaches its peak value of 2.45, after which the sample entered into strain softening zone. Similarly, the void ratio of the sample is plotted against axial strain (shown in Fig. 11). The void ratio also followed a typical trend of first decreasing and then dilating (e.g. Poulos 1971;De Josselin de Jong 1976; and Joseph 2012). After crossing 7% axial strain, the void ratio became almost constant at 0.775.

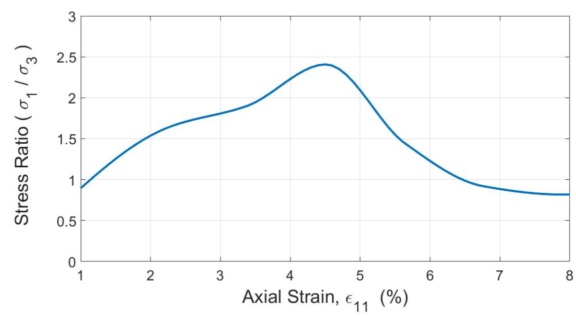

Fig. 10: Stress Ratio versus Axial Strain

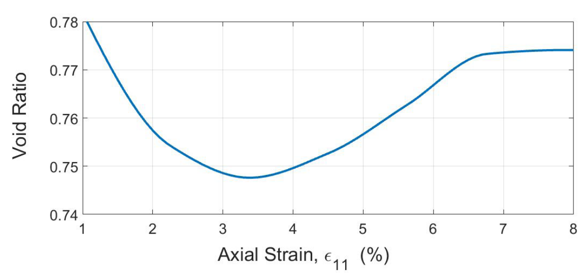

Fig. 11: Void Ratio versus Axial Strain

5. Conclusions

Knowing the importance of the granular media and an ongoing struggle to understand its interacting mechanism, an attempt has been made in terms of a numerical model to simulate three dimensional interactions of spherical soil particles. As convention, the model is attested for basic law of energy conservation and confirmation to envisage elastic and visco-elastic behavior of complex granular media before leading to perform a plain strain compression test on a three dimensional specimen.

The proposed numerical model successfully models the contacts between particles as pure elastic and visco-elastic. A particle with an initializing force follows a typical trend and keeps on oscillating in case of pure elastic contact model, whereas it attenuates when damping is applied. The system also shows a strong affirmation to law of conservation of total energy.

Finally, a plain strain compression test is performed to a three dimensional specimen of spherical balls with and without pre-consolidation pressure by using different combinations of flexible and rigid boundaries. During pre-consolidation, the velocity of particles sharply decreases to zero value after a number of iterative calculations which suggest a rigid pack by making solid contact between neighboring particles.

In plain strain compression on a pre-consolidated sample, the stress ratio first increases with axial strain until it reaches its peak value of 2.45, after which the sample entered in the strain softening zone and is well consistent behavior of granular media. The void ratio of the sample also follows a typical trend of first decreasing and then dilating. After crossing 7% axial strain, the void ratio became almost constant at 0.775.

References

[1]. Abdalsalam, M., and Gutierrez, M., 2010. "Comprehensive study of the effects of rolling resistance on the stress–strain and strain localization behavior of granular materials", *Granular Matter,* 12, 527–541.Catherine, O., 2011. "Particulate Discrete Element Modelling: a Geometric Perspective", *London and New York, Spon Press.*

[2]. Cleary, P.W., 2004. "Large scale industrial DEM modeling", *Engineering Computations*, 21(2/3/4), 169–204.

[3]. Cundall, P.A., 1971. "A computer model for simulating progressive large-scale movements in block rock mechanics", *Proc. Symp. Int. Soc. Rock Mech. Nancy, p. 2*

[4]. Cundall, P.A., 1988a. "Formulation of a three-dimensional distinct element model – Part I: a scheme to detect and represent contacts in a system composed of many polyhedral blocks", *International Journal of Rock Mechanics and Mining Sciences &Geomechanics Abstracts* 25(3), 107-116.

[5]. De Josselin de Jong, G., 1976." Rowe's stress - dilatancy relation based on friction", *Geotechnique,* 26(3), 527-534.

[6]. Iwashita, K. and Oda, M., 1998. "Rolling resistance at contacts in simulation of shear band development by DEM", *Journal of Engineering Mechanics* 124(3), 285-292.

[7]. Iwashita, K. and Oda, M., 2000. "Micro-deformation mechanism of shear banding process based on modified Distinct Element Method", *Powder Technology* 2(1), 192-205.

[8]. Joseph, P. G., 2012. "Physical Basis and Validation of a Constitutive Model for Soil Shear Derived from Micro-Structural Changes", *International Journal of Geomechanics,*13(4), 365–383.

[9]. Kozicki, J. and Dons, F.V., 2008. "YADE-OPEN DEM: an open-source software using a discrete element method to simulate granular materials", *Engineering computations,* 26, 7-26.

[10]. Lunding, S., 2008. "Introduction to discrete element methods: Basics of contact force models and how to perform the Micro-Macro transition to continuum theory", *EJECE-12/2008. Discrete modeling of geomaterials*, 785 – 826.

[11]. Mahmood, Z., Iwashita, K., 2009. "Influence of particle shape on shear band formation of quasistatic granular media", *Journal of Applied Mechanics, JSCE,* 12, 481–488.

[12]. Mahmood, Z., Iwashita, K., 2011 "A simulation study of microstructure evolution inside the shear band in biaxial compression test", *International Journal of Numerical and Analytical Methods in Geomechanics,* 35(6), 652–667.

[13]. Oda, M., Nemat-Nasser, S., and Konichi, J., 1985. "Stress-Induced Anisotropy in Granular Masses", *Soils and Foundations,* 25(3), 85–97.

[14]. O'Sullivan, C., Bray, J., and Cui, L., 2006. "Experimental Validation of Particle-Based Discrete Element Methods" *GeoCongress* : 1-18.

[15]. Pengcheng, F. and Yannis, F. D., 2012. "Quantification of large and localized deformation in granular materials", *International Journal of Solids and Structures,* 49(13), 1741–1752.

[16]. Peters, B., and Dziugys, A., 2002. "Numerical simulation of the motion of granular material using object-oriented techniques", Computer Methods in Applied Mechanics and Engineering, 191(17), 1983-2007.

[17]. Poulos, S. J., 1971. "The Stress-Strain Curve of Soils", *GEI Internal Report*

[18]. Rowe, P., 1962. "The stress-dilatancy relation for static equilibrium of an assembly of particles in contact", *Proceedings of the Royal Society of London. Series A, Mathematical and Physical Sciences* 269 (1339), 500–527.

[19]. Starck, D. L. and Cundall, P. A., 1979. "The Distinct Element Method as a Tool for Research in Granular Media", *Report to the National Science Foundation* (ENG76-20711).

[20]. Thornton, C., 2000. "Numerical simulations of deviatoric shear deformation of granular media", *Geotechnique* 50(1), 43–53.