CHAPTER 4
MODELLING FOR PARTICLE CHARACTERISTICS

4.1 MODELING OF STIFFNESS

4.1.1 INTRODUCTION
Granular media show considerably non-linear deformation behaviours due to evolution and collapse of microstructures formed in granular media during the macro behaviours. The mechanical behaviours of granular media are dependent strongly on density and stress history (including stress level) conditions. Moreover, even if they are under same condition, the mechanical properties of soils with different grain sizes, grain stiffness and grain shapes should be intrinsically different. In geo-mechanics and geo-engineering, the differences in stiffness with different sands and gravels, the density and stress-level dependencies of stiffness are very important properties which must be taken account for modelling the problems.

Grain properties influence macro deformation properties thorough a variety of stability against slip and deformability at contact points. In a series of papers (Maeda et al. 1995, Miura et al. 1997, Miura & Maeda 1999a,b, Miura et al. 1997, 1998), the relationships between physical and mechanical properties with variations in confining stress and relative density were investigated extensively for granular samples with different primary properties (e.g. density, hardness, grain shape and grain size). From test results, it was revealed that the primary and physical properties of sand significantly influence its mechanical behaviour and some reliable mutual relationships of physical and mechanical properties were identified. An estimation method of mechanical properties from some index physical properties was also discussed. Void ratio extent (e_max-e_min) which increases with increasing angularity of grain shape and decreasing grain size, was selected as a promising parameter for evaluating the ductile deformability, the degree of confining stress and relative density dependencies. In that paper series, it was indicated that grain crushability, which increases with angularity and grain size, also induces further reduction of shear strength with increasing confining stress. It can be said that grain shape brings both effects of unstable contact configuration and interlocking into the structural stiffness of microstructure composed of grains. Therefore, the effects of grain shape on the deformation-failure behaviours of granular material should be taken into account when simulating the ductile and compressive deformation behaviour of soils by the Discrete Element Method (DEM). Thus we employed non-circular particle elements in this paper to discuss macro stiffness properties by DEM.

The macroscopic behaviour of granular materials is controlled by evolution and collapse of microstructures. Stress-induced anisotropy in granular materials under shear has been observed in model tests and simulations (e.g. Oda et al. 1985), and elastoplastic models with an assumption, Chang (1988) and Chin and Chang (1990) proposed a relation among micro stiffness, arrangement of particles and macro stiffness by the followings,

\[ C_{ijkl} = \frac{1}{2V} \sum_n \sum_m f_{ij}^{nm} K_{ij}^{nn} t_{kk} \]

\[ K_{ij}^{nm} = k_s n^n_j n^n_i + k_t \tau^{ij} \tau^{ij} \] (for 2d)

where \( V \) is representative volume of the packing and \( t_{ij}^{nm} \) is the branch vector \( y^n_i - y^n_j \) joining the centres of particles \( n \) and \( m \) in contact. The contact stiffness tensor \( K_{ij}^{nn} \) can be obtained by contact stiffness (spring) \( k \)

Since we must solve many complex phenomena in geomechanics, it is clear that we must develop constitutive model based on micromechanics taking account for grain properties and the geometric parameters such as the fabric tensor of stress-induced anisotropy, the coordinate number and so on.

The purpose of this paper is to introduce the simulation results about the relationships among macro deformation properties (stiffness) of granular media, grain properties (stiffness, shape) and void ratio in bi-axial compression test (Maeda et al. 2003), and then discuss usability of DEM simulation taking account for effects of grain properties so as to solve further geo-engineering problems.

4.1.2 STIFFNESSES IN DESCREE MODEL

Micromechanical relations in micro-macro stiffness
In this subsection, the relation among contact stiffness (spring coefficients in DEM) in micro-scale, structural stiffness of microstructure in meso-scale and macro stiffness of continuum in macro-scale shall be concerned as shown in Fig.1.

Figure 4.1.1. Modelling of stiffness of granular media in multi-scale views.

Many researches about micromechanics of granular media have been conducted (reviewed by e.g. Oda & Iwashita, 1999). For example, on the basis of the micro structural continuum model with the uniform strain assumption, Chang (1988) and Chin and Chang (1990) proposed a relation among micro stiffness, arrangement of particles and macro stiffness by the followings,
and the vectors and $n'_j$ normal and tangential $t'_j$ to the contact plane, respectively.

From these equations, we can understand that the magnitude of stiffness is influence by that of tangential stiffness value $k$ of both contact spring elements, and Poisson's ratio described by ratio of stiffness tensor components also is varied by $k_n/k_t$. In the case of contact between circular particles, the direction of $n'_j$ is coincident with that of $t'_j$. Otherwise, for the case of non-circular particle, the vectors have difference in direction and thus normal contact force $f_n$ also mobilizes couple force around the particle. Therefore, this couple force must induces interlocking, unstable contacting and breakage of corner of particle. These effects are controlled not only by properties of the particle but also packing and stress condition, indicating that grain shape effect is not a material constant but a variable; the attribution of grain shape to stress-strain could be called structural stiffness.

The tensor $n'_j n'_i$ in this model relates with fabric anisotropy. The stress-induced anisotropy can be investigated based on the fabric tensor (Satake 1982), as defined by.

$$F_j = \frac{1}{2M} \sum_{ji} n'_j n'_i s_{ni} n'_j n'_i \tag{4.1.3}$$

where $M$ is the total number of contact points. The tensor is symmetric and the major and minor principal values are denoted by $F_1$ and $F_2$, respectively. In the same manner, a tensor can be defined for unit vector of branch vector $b = \mathbf{l}/|\mathbf{l}|$ by,

$$B_j = \frac{1}{2M} \sum_{ji} b'_j b'_i s_{b} b'_j b'_i \tag{4.1.4}$$

This tensor could be called 'branch fabric tensor'.

In Eq. (4.1.1), the summation $1/2V \Sigma$ for contact points is associated with coordinate number $N_c$ statistically, which is averaged number of contact in REV. We could think $N_c$ as an index of stability of force transmission path (e.g. Kuwabara and Maeda, 2000; Kuwabara et al. 2002).

For the above reason, we must need the relation among anisotropies, $N_c$ and grain properties based on micromechanica consideration on modelling of stiffness.

Contact stiffness: spring elements

The deformation behaviour of granular material was analyzed by the DEM (Cundall and Strack 1979). The equilibrium contact forces and displacements of grains in the stressed assembly were calculated individually at small time steps on the basis of Newton’s second law. The interactions between elements were modelled by contact elements between rigid disks (e.g., springs, dash-pots, sliders and non-extensional elements), as shown in Fig. 4.1.2a and b.

![Figure 4.1.2. Contact elements at contact points in DEM: (a) normal direction, (b) tangential direction.](image)

All calculations in 2D DEM were conducted with force-displacement laws described by solid line in Fig.4.1.3. Particles are treated as rigid bodies but allowed to overlap another one at contact points by soft-contact algorithm, where overlaps are very small compared with particle size. The contact forces are related to the magnitude of the overlaps as sown in Fig.4.1.3. Tangential force increases in proportion to displacement along $k_t$ when the force does not attach the yield condition. Otherwise, when the yield condition is being hold, the force does not increase: this is stable sliding. Once the sliding condition is violated, the stiffness against shearing at contact point recovers. This mechanism influences the elastic and plastic behaviours of granular media; we must note, however, that so-called macro elastic behaviour must not be equal to summation of displacements in springs, but mainly controlled by change in the number of contact points at sliding and collapse-regeneration of microstructures. Future, we might consider strain softening to improve the precision of simulation.

![Figure 4.1.3. Force-displacement laws at contact point described by normal and tangential springs $k_n$ and $k_t$: contact forces $f_n$ and $f_t$ versus displacements $\delta_n$, $\delta_t$.](image)

The spring coefficient in the case of only true sphere or circular grains could be estimated by the Hertz-Mindlin contact model which explains a nonlinear contact response by an approximation of the elastic theory of Mindlin and Deresiewicz (1953) and Cundall (1988). Hakuno (e.g. Hakuno et al., 1991; Hakuno et al., 1997), moreover, proposed that we could determine spring coefficients as a first trial value by using the following equations, and then changing them to be suited to our model by trial and errors.

$$k_n = \pi/4 \cdot \rho \cdot V_n^2 \tag{4.1.5a}$$

$$k_t = \pi/4 \cdot \rho \cdot V_t^2 \tag{4.1.5b}$$
\[ \frac{V_p}{V_s} = \sqrt{\frac{2(1-\nu)}{1-2\nu}} \]  

(4.1.5c)

where \(V_p\) and \(V_s\) are velocity of compression and shear wave in isotropic granular material, respectively, and \(\rho\) is density of granular material with Poisson's ratio \(\nu\). The above equation was derived by finite differential equation of 1D wave propagation in lattice composed of particles. If \(\nu = 1/3\) in Eqs.(4.1.5), ratio of spring coefficients \(k_t/k_s\) will be 4.

**Structural stiffness: non-circular particles**

As mentioned above, grain shape plays an important role on deformability or stiffness of microstructure. This stiffness, however, is not material constant and is varied by change in arrangement of particle and stress condition. Circular (Fig. 4.1.4a) and non-circular (Figs. 4.1.4b-e) particle elements are considered in this paper. For example, the non-circular particles shown in Fig. 4.1.4b were prepared by connecting three circular particles of the same radii as a "clump particle". Particles were generated for a material composed entirely of circular particles, and then all circular particles were replaced by non-circular particles, where the circular particles are shown as broken lines in Figures 4.1.4(c), (d) and (d) and circumscribe non-circular particles. The parameters for particle elements used are described in Table 4.1.1.

![Figure 4.1.4. Particles types used in the DEM: (a) c101 (circle), (b) c103 (triangle), (c) c104 (quadrate), (d) c106 (hexagon), (e) c108 (octagon), where broken line is circumscribing circle.](image)

**Table 4.1.1. Reference analysis parameters of particle elements.**

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Particle – Particle</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density (kg/m³)</td>
<td>2700</td>
</tr>
<tr>
<td>Diameters (mm)</td>
<td>5 to 10 (uniform frequency)</td>
</tr>
<tr>
<td>Normal Spring Coefficient (k_n) (N/m/m)</td>
<td>(5 \times 10^7(500M))</td>
</tr>
<tr>
<td>Tangential Spring Coefficient (k_t) (N/m/m)</td>
<td>(5 \times 10^7(500M))</td>
</tr>
<tr>
<td>Damping</td>
<td>Critical Damping</td>
</tr>
<tr>
<td>Resistive Friction Angle (\varphi)</td>
<td>(\tan \varphi_0 = 0.25) (Fric. coeff.)</td>
</tr>
</tbody>
</table>

**Macro stiffness: packing with density control**

Macro stiffness of the material is strongly influenced by density of assemble (specimen). It must be required to regulate mass density to hold the similarity law in mechanics between simulation model and practice problem (prototype model) in order to obtain good analysis results. The stiffness of sands, cobbles and gravels under any stress conditions are modelled on the basis of experimental results and theoretical speculation. We could know knowledge about experimental useful works and their recent mechanical interpretations by referring to books written by Ishihara (1996), P.H.R.I. (1997) and Wood (2004). Typical formulation is represented as a function of void ratio and stress condition by,

\[ \text{Stiffness} = A \cdot f(e) \cdot g(\sigma) \]

(4.1.6)

where \(A\) is reference parameter, and it is also influenced by grains shape.

Figures 4.1.5a and b show the specimen models employed for simulations of biaxial compression tests under isotropic compression and shear failure states. The analysis involved approximately 4000 disc particles and four wall boundary elements, the movement of which was employed for external stress and strain control, as shown in Fig. 4.1.5, where gray balls and black lines denote particles and the network of contact force transmission. The biaxial compression tests were simulated under zero gravity conditions to investigate the change in fabric due to the change in macro stresses.

![Figure 4.1.5. Specimens model for bi-axial compression test simulation by DEM: (a) isotropic stress, (b) shear failure.](image)

Specimens were prepared as follows. First, circular particles with initial resistance friction coefficient \(\tan \varphi_0\) were generated such that the porosity was equal to \(n_0\) in the region enclosed by the boundary walls. At \(n_0 = 0.40\), there were almost no contact points and initial packing was loose. At \(n_0 = 0.10\), there were many contact points and initial packing was dense. Each circular particle was then replaced by a clump particle with \(\tan \varphi_0\) using the procedure described in the previous subsection. After the initial stress was regulated to the required value of \(\sigma_{max}=k_s \cdot 10^{-4} (0.05MPa)\) by adjustment of the boundary walls, the stress condition was held for stabilization. Finally, the friction coefficient was shifted instantaneously from \(\tan \varphi_0\) to \(\tan \varphi\) (= 0.25 in this paper), and the initial void ratio \(e_0\) was obtained after stabilization under \(\sigma_{max}\).

Figures 6a and b show the change in the void ratio \(e_0\) with \(\tan \varphi_0/\tan \varphi\) for \(n_0 = 0.40\) and 0.10. The void ratio \(e_0\) increases with \(\tan \varphi_0/\tan \varphi\) and initial porosity.
On the basis of these results, the initial density of the specimen can be regulated easily by adjusting the resistant friction angle of particles and initial porosity. For a dense specimen, \( \tan \varphi_{\mu 0} \) is set at 0.0 and \( n_0 \) is set at 0.10, whereas for a loose specimen, \( \tan \varphi_{\mu 0} = 1.0 \) and \( n_0 = 0.10 \). Therefore, minimum and maximum mechanical void ratios \( e_{\text{max}} \) and \( e_{\text{min}} \) could be obtained by simulating both end conditions. The void ratios and the extent of void ratios \( (e_{\text{max}} - e_{\text{min}}) \) which is denominator of relative density \( D_r \) (referred to 4.1.1) are plotted in Fig.7; all void ratio parameters of non-circular particles show larger values (Maeda et al., 1997) than circular particle.

### 4.1.3 Macro Deformation Behaviours

**Macro deformation behaviours**

In this subsection, analysis results of biaxial compression tests by DEM using non-circular particle element. In the following subsections, stiffness properties are discussed.

### Table 4.1.2. Basic analysis cases of bi-axial compression tests.

<table>
<thead>
<tr>
<th>Grain Shape</th>
<th>Test under constant confining pressure</th>
<th>Test under constant volume</th>
</tr>
</thead>
<tbody>
<tr>
<td>Circular</td>
<td>( c_0 = 0.20 )</td>
<td></td>
</tr>
<tr>
<td>(Density)</td>
<td>( \sigma_0 = 2k_n \times 10^{-4} (0.1 \text{MPa}) )</td>
<td></td>
</tr>
<tr>
<td>Medium</td>
<td>( c_0 = 0.23 )</td>
<td></td>
</tr>
<tr>
<td>(Consolidation Stress)</td>
<td>( \sigma_0 = 2k_n \times 10^{-4} (0.1 \text{MPa}) )</td>
<td></td>
</tr>
<tr>
<td>Loose</td>
<td>( c_0 = 0.27 )</td>
<td></td>
</tr>
<tr>
<td>(Consolidation Stress)</td>
<td>( \sigma_0 = 2k_n \times 10^{-4} (0.1 \text{MPa}) )</td>
<td></td>
</tr>
<tr>
<td>Non-circular</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Dense</td>
<td>( c_0 = 0.20 )</td>
<td></td>
</tr>
<tr>
<td>(Density)</td>
<td>( \sigma_0 = 2k_n \times 10^{-4} (0.1 \text{MPa}) )</td>
<td></td>
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<td></td>
</tr>
</tbody>
</table>

Stresses were then varied to the prescribed consolidation stress. The analysis cases are shown in Table 2. Stresses \( \tau_{y} \), \( \sigma_{xy} \), \( \sigma_{yy} \), \( \sigma_{xx} \), \( \sigma_{mm} \), and \( \sigma_{mn} \) are the mean normal stress and maximum shear stress respectively; \( \sigma_{c0} \) is confining pressure which is \( \sigma_{mm} \) at initial state of shear. Normal strains in x and y axis and volumetric strain are denoted by \( e_{\text{xx}}, e_{\text{yy}} \), and \( e_{\text{v}} \) respectively.
Figures 4.1.9 and 4.1.10 show the confining stress dependence and density dependence of deformation behaviours in the case of an assembly of triangular particles (c103). The relationship between the void ratio and the mean normal stress under isotropic compression and shear also is presented in Figure 11. As observed in experiments (e.g. Fukushima & Tatsuoka 1984), the specimens with lower density exhibit a lower stress ratio at failure and higher contractive deformation under higher confining stress, indicating ductility.

As shown in Figure 4.1.11, there seems to be a critical state region (indicated by a broken line) in which the shear strain is large. However, the difference between the critical state lines for dense and loose specimens is significant. This indicates that since deformation localization tends to occur in dense specimens, it may be possible to investigate the relationships between the void ratio and the mean normal stress \( \sigma_m \) for both the specimen as a whole and locally in the shear band (for discussions on mechanical behaviours of micro zones in specimens refer to e.g. Desrues, 1996; Wong 1999; Maeda et al., 2003).

Figures 4.1.12a–c show the density dependence of deformation behavior under a constant volume condition, for non-circular particles (c103), corresponding to 'undrained test'; (a) stress ratio and strain, (b) reduction of effective mean normal stress, (c) stress paths.

Figures 4.1.12a–c show the density dependence of deformation behavior under the constant volume condition in terms of the stress-strain curve, the reduction in effective mean normal stress, and the stress path. In the case of the lowest density (\( e_0 = 0.27 \)), it can be found that brittle deformation occurs, causing fluid flow and reducing the effective mean normal stress remarkably. These tendencies indicate the occurrence of static liquefaction. This fluidity reduces with increasing density.

These tendencies of deformation failure have also been observed in experiments (Ishihara 1996). The density and stress level dependencies can therefore be simulated well through the use of non-circular particles.
in the DEM, demonstrating that grain shape represents an important factor determining the compressibility and ductility of soils.

**Micromechanical behaviours**

Here, observation results for fabric evolution are introduced.

It is known well that coordinate number $N_c$ increases with an increase in mean normal stress $\sigma_m$, and a decrease in void ratio. However, contrary to our expectation, we do not know properties of $N_c$ well during shearing. Figures 13 shows the changes in coordinate number $N_c$. The coordinate number decreases remarkably from 3–4 to about 2.5 with the progression of shear. When $N_c$ is less than 2.5, the stiffness remains low and is not restored. As the coordinate number appears to represent the stability and restorative ability of the contact paths, the specimen with high $N_c$ has a highly stable fabric (Oda 1997). Thus, $N_c$ indicates the degree of percolation of microstructures in granular media (the details were introduced by Ohmura (2005)).

$$F_1/F_2 = \sqrt{\sigma_1/\sigma_2}$$ (7)

Thus, it can be said that the evolution of stress-induced anisotropy is dependent on the square root of principal stress. This relationship is useful for developing a constitutive model. The relationship was first proposed by Satake (1982), and has subsequently been utilized for development of the concept of modified stress (Nakai & Mihara 1984; Tobita & Yanagisawa 1992). Otherwise, branch fabric tensor in Eq.(4) is influenced by grain properties and test conditions (e.g. Sakurai et al., 2005).

![Figure 4.1.13. Decrease in coordinate number with increasing shear deformation at constant volume.](image)

**Effects of contact stiffness**

Figures 4.1.15a-c show stress-strain-dilatancy behaviours of assemblies of circular particles with different contact stiffness under $\sigma_{0i}=0.5$MPa; $k_n=5 \times 10^6$ MN/m/m and ratios $k_n/k_i=0.1$–100 are varied. As shown in Fig. 15(a), macro stiffness and expansibility (positive dilatancy) increase with increasing $k_n$, but the peak strength almost does not change (in $k_n/\sigma_{0i}=2 \times 10^2$–$10^4$). When $k_n$ is extremely low (in other words, it is too lower than stress level such as $k_n/\sigma_{0i}=2 \times 10^2$($k_n=5 \times 1$ and $5 \times 10$MN/m/m), the macro behaviours are strange. From Fig. 15(b), the stiffness, moreover, changes with a variety of ratio $k_n/k_i$ (unfortunately, magnitude of spring coefficient also changes with the ratio). On the basis of stress-dilatancy plots in Fig. 15(c), in small strain range, expansibility increase with $k_n/k_i$. Otherwise, residual strength does not change even with different $k_n/k_i$. Especially in small strain, the ratio is very important.

In Sec. 5.3 in this report, these effects of contact stiffness on macro deformation-failure properties are discussed in detail for application to a rubble mound.

**Effects of structural stiffness (non-circular elements)**

Figure 16 shows stress-dilatancy behaviours (flow rule) in pre-failure state with different grain shapes for dense packing. We can see nonlinear relationships between stress ratio and dilatancy. The dilatancy factor $d\varepsilon_d/d\varepsilon_\alpha$ at initial state are different with grain shape. Under high stress ratio (from zero volume increment state to failure state) the behaviour are different. Even if friction coefficient $\tan \phi_b$ is same, granular materials with different grain shape have different stress ratios at zero volume increment state and different increment ratio of stress ratio-dilatancy. The values for non-circular particles are higher than that for circular particle. This tendency shows that dilatancy property and ductility should be depend on $(\varepsilon_{max}-\varepsilon_{min})$ in Fig. 4.1.7, implying that dilatancy properties (compressibility and interlocking) could be modelled by quantifying grain shape on the basis of micromechanics.
4.1.4 CONCLUSION

The usefulness and the validity of DEM with non-circular grains were presented focused on stiffness properties of granular media in bi-axial tests. By conducting element tests with DEM, we can investigate relationships between macro stiffness and evolution rule of microstructure (e.g. stress-induced anisotropy, interlocking effect and so on). In this paper, the unique relationship between fabric tensor and principal stresses as described in Eq.(7), dependent of grain properties and test condition were revealed. In addition, dilatancy properties and ductility are influenced by $(e_{\text{max}} - e_{\text{min}})$.

On the basis of a series of analysis, it was shown qualitatively and clearly that macro stiffness or deformability is influenced by not only micro contact stiffness (spring coefficient) but also structural stiffness (interlocking or grain rolling resistance). By using non-circular particle element and improving procedure of packing, we can, moreover, control density of assemble extensively and can thus explain ductile and compressive deformation-characteristics including density and stress-level dependencies of stiffness.

These results indicate that we can, easily and properly, simulate both of stiffness and strength of material or ground; the similarity between a simulation model and a practical problem (prototype model) become to be satisfied. Modelling stiffness in DEM using non-circular element (or numerical algorithm with equivalent characteristics to it) make DEM very useful tool for further geo-engineering problems.

Effects of packing density

Stiffness which is calculated by $\frac{\Delta \sigma_{c}}{\Delta e_{2D}}$ at strain $e_{\text{2D}}=1 \times 10^{-4}$ under $\sigma_{c}=0.1$MPa is plotted against void ratio $e$ at initial state of shearing in Figure 4.1.17. It can be said that stiffness is determined as a function of $e$ as introduced by Ishihara (1996), P.H.R.I. (1997) and Wood (2004).

Figure 4.1.17. Decrease in macro stiffness with an increase in void ratio in the cases of circular particles and non-circular particles under $\sigma_{c0}=0.1$MPa.

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4.2 MODELING OF IRREGULAR GRAIN SHAPE OF SAND

4.2.1 INTRODUCTION

A rapid increase of computer abilities in the recent past has drastically extended the availability of Discrete Element Method (DEM). Recently, in the field of soil mechanics, some researchers attempted so-called ‘virtual’ element tests such as a tri-axial compression test with DEM (Thornton and Liu 2000, Muhlhaus, H.-B. et al. 2001). They dealt with a considerable number of 3-D particles (5000 to 10000) to obtain more realistic simulation results. However, it is still difficult to compare such DEM results quantitatively with physical experimental results of real sand mainly because of the lack of adequate grain-shape modeling. Natural sand grains have very complicated shapes necessarily affect the macro behavior (stress-strain curve, dilatancy curve, etc.) of an element test specimen. It seems true to say that angular grains have much higher shear strengths than roundish grains, but the mechanism is still not clear and quantitative estimations have not been successfully made yet.

In order to study this grain-shape effect, several researchers have conducted Discrete element simulations with non-circular (or non-spherical) particles. Rothenberg and Bathurst (1992) conducted a series of bi-axial test with elliptic elements of different aspect ratios and showed that the maximum shear strength was exhibited with a specimen composed of ellipses whose aspect ratio was around 0.8. Mirghasemi et al. (1997) dealt with polygonal particles in order to study the effect of confining pressure on peak shear strength, but grain-shape effects were not discussed in depth. Matsushima and Konagai (2001) simulated a series of simple shear tests with 2-D elliptic elements and regular polygonal elements to discuss the grain shape effect in detail. It was demonstrated in their study that regular polygonal elements exhibit larger rotational resistance at their contact points, which leads to higher shear strength. They also conducted grain shape analysis for four different sands, and suggested that the mechanism of grain-shape effect of real sands may be similar to that of regular polygonal elements.

In relation to the rotational resistance at the contact points, Iwashita and Oda (1998) proposed a DEM with circular elements in which an additional rotational spring is assumed at each contact point. This is considered as a indirect but efficient approach to include the effect of grain shapes into DEM, though further study between rotational resistance and grain shape is needed.

In an attempt for a 3-D non-spherical element, Lin and Ng (1997) and Ng (1999) proposed the DEM with ellipsoidal elements and Ghaboussi and Barbosa (1990) formulated polyhedron DEM, but they didn’t discuss the connection to real grain shapes.

Considering these circumstances, it appeared worth conducting discrete element simulation with grains whose shapes were directly modeled from real sand grains. This study deals with such direct grain-shape modeling by a combination of primitive circular or spherical elements. A newly developed algorithm enables us to find the optimum sizes and positions of primitive elements for describing a complicated grain shape. Its concept is quite simple, and is easily applicable not only in 2-D but also in 3-D modeling. Accuracy and convergence of this algorithm are discussed in detail in this paper. Then the adaptability of the modeled grains into DEM simulations was studied through an element test. Based on the simulation results, the grain-shape effect in such granular materials as sands is then discussed.

4.2.2 DYNAMIC OPTIMIZATION FOR GRAIN SHAPE MODELING

Basic algorithm

The proposed algorithm is called dynamic optimization; because the optimized solution is obtained through a virtual time-marching scheme. First we assign the number of primitive elements used for the modeling, and set arbitrary initial sizes and locations. Usually the initial size is set to be sufficiently small in comparison with the size of the target grain and the initial locations are assigned inside the target grain. Then, we assume a kind of virtual force acting on the primitive elements. This force is an attraction from the surface of the target grain. The surface of the target grain is given as a set of discrete points, and the attraction directs from the centroid of the primitive element to each surface point (Figure 4.2.1(a)(b)). The magnitude of the attraction is proportional to the distance between the primitive element and the surface point.

When plural primitive elements are adopted, it is assumed that the attraction of each surface point acts only on the element closest to the point (Figure 4.2.1(c)). More exactly, the following value \( \delta^j \) is checked for each element \( i \):

\[
\delta^j = d^j - r^j
\]  

(4.2.1)

where \( d^j \) is the distance between \( j \)-th surface point and the centroid of \( i \)-th element, and \( r^j \) is the radius of the element. Then the element which has the

![Figure 4.2.1 concept of a virtual force acting on the elements](image-url)
minimum \( \delta^i \) is chosen as the representative element of this surface point, and the following attraction is applied to the element:

\[
f^i = k(d^i - r^i)
\]

where \( k \) is a spring constant. The attraction is directed from the centroid of the element to the surface point when \( f^i \) is positive.

By summing all the attractions, each element moves and expands (or shrinks) according to a virtual equation of motion. By introducing an additional damping in the equation of motion, the motion of the elements is converged after some calculation steps. In this converged configuration, the equilibrium has been met in each element for both volumetric and translational components. This final configuration of the elements is then the optimum solution in this algorithm.

The algorithm is summarized in a flow chart (Figure 4.2.2).

2-D modeling

Figure 4.2.3(a)(b) show an example of the 2-D converging process with a single circular element. It is clear that the element approaches to the converged solution with some oscillation. It is necessary to set adequate parameters (spring constant and damping coefficient) for the rapid convergence. Figure 4.2.3 (c) shows that a unique solution is obtained wherever the initial position of the element is assigned (cross marks in the figure show the randomly-assigned initial positions).

When plural primitive elements are adopted, however, the converged solution is not unique but is strongly influenced by the initial configuration. Figure 4.2.4 shows two different converged solutions that are obtained from 10 different initial configurations with two elements. To judge the accuracy of the converged solution, the following error index is introduced:

\[
err = \frac{1}{N} \sum_{j=1}^{N} |d^j - \bar{r}^j| 
\]

where \( N \) is the number of surface points of the target grain, \( R_{eq} \) is the radius of the circle whose area (or volume in 3D) is equivalent to the one of the target grain, \( d^j \) is the distance between the \( j \)-th surface point and the centroid of the element representing this surface point, and \( \bar{r}^j \) is the radius of the element.

Since it is difficult to find the theoretical optimum solution, we currently repeat a sufficient number of calculations with different initial positions, and the most accurate solution is chosen based on the error index.

When the number of adopted elements is increased, another problem arises; some of the elements come fully inside another element and become inactive. To avoid the degradation of the solution by these inactive elements, it is effective to introduce an additional scheme that such elements are re-located around the most-inaccurate surface point. Figure 4.2.5 shows an example obtained with ten elements, which seems to attain sufficient accuracy of overall grain shape. It should be noted that this modeling cannot describe the
small surface roughness of real sand grains. However, this surface-roughness effect may be incorporated into DEM simulations by changing the friction coefficient. Figure 4.2.6 shows the convergence with a different number of primitive elements. Convergence becomes worse with larger numbers of elements and the curves are jagged (not monotonic). This is due to the fact that the change of the elements’ configurations causes a change of the mathematical problem itself; the connection of virtual springs between the elements and the grain surface points are determined by the current configuration of the elements.

Figure 4.2.7 shows the relation between the final error index and the number of adopted elements. The final error index is determined as the value after a sufficient number of calculation steps. Certainly, a better result is attained with larger number of elements, but the increase of the number of elements leads to the increase of the computation time in DEM simulation. Therefore, an adequate number of elements for the modeling should be chosen taking account of both the accuracy and the computational efficiency in DEM simulation.

3-D modeling

It is straightforward to apply the above algorithm into 3-D modeling. However the number of elements required to satisfy a certain accuracy becomes much larger. Figure 4.2.8 shows an example of 3-D grain modeling with 100 elements. The obtained error index is err=0.00962 which is comparable to that of 2-D modeling with 10 elements (err=0.00970), though the target grain shape is completely different. From a dimensional consideration, the accuracy with N elements in 2D is same as that with $N^2$ elements in 3D. According to Figure 4.2.6, the accuracy with smaller elements does not obey this rule, mainly due to the difference of the target grain shape, but the accuracy with a larger number of elements seems to be in good agreement with the rule. Therefore we can choose the number of primitive elements used for the representation of one grain based on Figure 4.2.6.

4.2.3 APPLICATION TO DISCRETE ELEMENT METHOD

2-D simulation

A series of 2-D simple shear simulation by DEM are presented in this section. 50 grains are modeled for Toyoura sand and Ottawa sand, respectively, and the modeled grains are duplicated 4 times to make a specimen with 200 grains (Figure 8(a)(b)). Each grain is modeled with 10 circles. According to the conventional classification, Toyoura sand is sub-angular and Ottawa sand is sub-rounded, but it is hard to recognize this difference only by the visual
impression of Figure 4.2.8. Physical experiments by Yoshida and Tatsuoka (1997) shows that Toyoura sand has higher peak strength than Ottawa sand. DEM parameters used in this section are listed in Table 4.2.1. Grain size distributions for the two specimens are shown in Figure 4.2.9, which are in good agreement with the measurement. Several specimens were prepared by the vertical compaction with different interparticle friction angles so as to make their initial void ratios different. Periodic boundary is set to both sides of the specimens, and the grains around the top and the bottom boundaries are rigidly connected one another to make frictional planes sandwiching the rest of the grains. Under a constant confining pressure, lateral displacement is imposed at the bottom plane. Figure 4.2.10(a) and (b) show the snapshots of the specimen before and after the shear deformation, respectively for a dense specimen of Toyoura sand. It is shown that a localization of deformation takes place in the specimen. Figure 4.2.11 shows the evolution of mobilized friction angle accompanied by the imposed shear strain for Toyoura sand model and Ottawa sand model. In this figure the result by an equivalent circles model (whose volume distribution is exactly equal to the Toyoura sand model) is also plotted. All specimens have the similar void ratio of about 0.20. It is clear that

Figure 4.2.8 Modeled grains

(a) Toyoura sand model

(b) Ottawa sand model

Table 4.2.1 DEM parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Grain density</td>
<td>2.64 (g/cm²)</td>
</tr>
<tr>
<td>Spring constant (normal)</td>
<td>1.0e9 (g/s²)</td>
</tr>
<tr>
<td>Spring constant (tangential)</td>
<td>2.5e8 (g/s²)</td>
</tr>
<tr>
<td>Damping coefficient (normal)</td>
<td>2.0e2 (g/s)</td>
</tr>
<tr>
<td>Damping coefficient (tangential)</td>
<td>1.0e2 (g/s)</td>
</tr>
<tr>
<td>Friction coefficient between grains</td>
<td>27 (deg.)</td>
</tr>
<tr>
<td>Time increment</td>
<td>2.5e-8 (sec.)</td>
</tr>
</tbody>
</table>

Figure 4.2.9 Grain size distribution of modeled grains

Figure 4.2.10 Snapshots of the specimen (Toyoura sand, dense)

(a) Before shear

(b) After shear

constant confining pressure

periodic boundary
Toyoura sand model has higher peak strength than Ottawa sand model, and the circles model has much lower peak strength than both sand models, which is consistent with physical experiments (Yoshida and Tatsuoka 1997). One can see this tendency more confidentially with Figure 4.2.12 that shows the peak strength with respect to the initial void ratio for the three models. Since other grain parameters are totally same, this difference in shear resistance clearly comes from the difference in grain shape. Therefore, the proposed direct modeling method works well so that Toyoura sand model exhibits higher peak strength than Ottawa sand model.

The mechanism of grain shape effect on shear strength can be explained as follows. Many sand grains are in contact with each neighbor not at single point but at two or more points as shown in Figure 4.2.13. In the figure the segments connecting the grains indicate the contact forces and the thicker segments show the larger forces. These plural contact points allow transmitting moment between the contacting grains and resisting their relative rotation, which leads to the increase of shear strength (Figure 4.2.14). This mechanism was pointed out by Matsushima and Konagai (2001) through the simulation with regular polygonal elements.

One can easily realize that the possible void ratio range in 2-D model, as shown in Figure 4.2.10 cannot be compared directly with the 3-D void ratio range. Therefore, for quantitative discussion, it is necessary to conduct 3-D simulations as described in the next section. However, it should be noted that 2-D simulation is worth conducting for exploring the essence of granular materials.

**3-D simulation**

Some 3-D simple shear simulations are presented in this section. 400 Toyoura sand grains are modeled from the data of micro X-ray CT experiment (Matsushima et al. 2004). Each grain is modeled with 10 spheres. Figure 15 shows the grain size distribution of the modeled grains. Comparing with Figure 4.2.9 one can recognize that the grain size is relatively large, which is mainly because of the inaccuracy of the grain shape data itself.

DEM parameters used in this section are listed in Table 2. Spring constants are much smaller than 2-D case, for the computational efficiency, which means that the grains are much softer than the real sand grains.
Specimen has 1.5mm wide, 1.5mm deep and about 1.1 mm high. Smooth flat plates are set in front and back of the specimen to realize a plane strain condition, while periodic boundary is assumed on its left and right side (Figure 4.2.16(a)). Specimens with various void ratios are prepared under gravity field by changing the interparticle friction angle. After stabilization, the grains around the top and the bottom edges, respectively, are connected to make rigid frictional plates sandwiching the specimen. A confining pressure of 1.0 kPa is then applied through the plates. Stress-strain curves and dilation curves for the specimens with various initial void ratios are summarized in Figures 4.2.17 and 18, respectively. These figures include some experimental results of hollow-cylindrical torsional simple shear test of Toyoura sand (Pradhan et al. 1988). Simulation results are in good agreement with the experimental results in a quantitative way. It is worth mentioning that the results shown in the figures are based on the macroscopic (overall) strain measure. Therefore the responses after the yield state are strongly affected by the size of the specimen because of the strain localization. Since the height of the DEM specimens

Table 4.2.2  DEM parameters used in this section

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density of grain</td>
<td>2.64 g/cm³</td>
</tr>
<tr>
<td>Spring constant (normal)</td>
<td>1.0e6 g/s²</td>
</tr>
<tr>
<td>Spring constant (shear)</td>
<td>2.5e5 g/s²</td>
</tr>
<tr>
<td>Damping coefficient (normal)</td>
<td>2.0e-2 g/s</td>
</tr>
<tr>
<td>Damping coefficient (shear)</td>
<td>1.0e-2 g/s</td>
</tr>
<tr>
<td>Friction coefficient (tan ( \phi ))</td>
<td>0.51 (( \phi ) = 27 deg.)</td>
</tr>
<tr>
<td>Time increment</td>
<td>5.0e-5 s</td>
</tr>
</tbody>
</table>

Figure 4.2.15 Grain size distribution of modeled grains

(a) before shear

Figure 4.2.16 Snapshots of the specimen (Toyoura sand, dense)

(b) after shear (shear strain = 25%)

Figure 4.2.17 Evolution of stress ratio

Figure 4.2.18 Evolution of volumetric strain
are much smaller than those in experiments, the strain softening rate in the simulation becomes much milder. Also, the considerably large volumetric strain in the simulations is due to the specimen size.

Figure 4.2.19 shows the internal friction angle with respect to the initial void ratio of the specimens. The figure includes the TSS test results by Pradhan et al. (1988). Additionally, some DEM results of spheres are put together for reference. Note that the internal friction angles in the figures are computed by \( \phi_d = \tan^{-1}(\tau/\sigma_n) \). The figure clearly indicates that the result in Toyoura sand DEM with the interparticle friction angle of 20 degrees is quite close to the experimental result.

4.2.4 SUMMARY

Particle shape is of primary importance on the mechanical behavior of engineering granular materials. This article overviewed the methodology to incorporate the irregular shapes of the real materials into Discrete Element simulation, which is termed image-based modeling. The proposed method was validated through 2-D and 3-D simulations of the standard sands, though further investigation is necessary to achieve the better accuracy. In any cases, this kind of approach is essential to perform high-quality Discrete Element simulations.

REFERENCE


Rothenburg and Bathurst (1992), Micromechanical features of granular assemblies with planner elliptical particles, Geotechnique, 42(1), 79-95.


4.3 MODELING OF CRUSHABLE SOIL

4.3.1 INTRODUCTION

DEM simulation of perfectly elastic and infinitely strong grains provides many insights into the deformation of granular media (Thornton, 2000). Qualitative agreement of the mechanical behaviour between the simulated results and real sand was found, yet the stress level dependency of granular behaviour could not properly be represented because the crushability of sand was ignored. The use of DEM in modelling the behaviour of crushable soil has aroused increasing attention since the crushability of soil grains was included in the modelling procedure. Following Robertson (2000), numerical ‘grains’ (agglomerates) can be made by bonding elementary spheres in probabilistically flawed ‘crystallographic’ arrays. McDowell and Harireche (2002) also validated the use of DEM in modelling soil particle fracture. Not only could DEM simulate the crushing strength of a real sand grain, with diametral breakage of the bonded agglomerates between flat platens, it could also reproduce realistic Weibull distributions of crushing strength in a batch of flawed agglomerates. Cheng et al. (2003) applied this DEM approach to simulate the compression and shearing behaviour of an element of crushable soil (silica sand) by reproducing the statistical crushing strength of a batch of uniformly sized ‘grains’ randomised by the removal of 20% of the micro-spheres. Reasonable agreement was found between the real data obtained from isotropically compressed silica sand and the DEM simulation when stress was normalised by the characteristic crushing strength of the grains. Cheng et al. (2004) had the foregoing research with particular focus on the fundamentals of yielding and plastic deformation. The purpose of this paper is to introduce the simulation result by Cheng et al. (2003, 2004), and to justify the use of the modelled grains in further geotechnical engineering applications.

4.3.2 MODELLING OF CRUSHABLE GRAINS

Arraying and bonding of spheres

Grains were made from a regular assembly of spheres in hexagonal close packing (HCP), without initial overlap. As these agglomerate grains were intended to represent solid particles, the main purpose of the regular packing was to minimise the space between the balls of the agglomerate. A stiffness model, a bonding model and a slip model are included in the constitutive representation of contact points between the elementary spheres. The bonding model serves to limit the total normal and shear forces that the contact can carry by enforcing bond-strength limits. The maximum tensile force that the bond can sustain in tension and the maximum shear force it can withstand before breaking are specified when the bond is created. The bond breaks if either of these values is exceeded. Following Robertson (2000), the parameter on the agglomerate grain, which models the properties of a typical sand grain was given. The contact normal and shear stiffness and the contact bond strength of each micro-sphere, 0.2 mm in diameter, were 4 MN/m and 4N respectively. The frictional coefficient at the surface of the micro-sphere is 0.5, equivalent to $\theta = 26.6^\circ$. In order to provide a statistical variability to strength and shape of the agglomerates, similar to that of a real sand, each elementary sphere of an agglomerate was given a probability of existence of only 80% when it was created. As a result an average of 20% of the elementary spheres will not appear in the final agglomerate used for subsequent testing, about 11 balls less than the maximum number of 57 as shown in Figure 4.3.1.

Figure 4.3.1 Examples of DEM agglomerate grains (Cheng et al, 2003)

Mechanical behaviour of modeled grains

Randomly-orientated agglomerates were then numerically crushed between two smooth and stiff platens under strain-controlled compression. This is similar to the procedure described by Robertson & Bolton (2001). The initial separation of the platens was the same as the size of the agglomerate, which is 1.0 mm. With the variability given to the agglomerates, different peak strengths were obtained from 20 tests. Figure 4.3.2 shows a typical result from the crushing tests; it is compared with the crushing of a silica grain reported by Nakata et al (2001). The diameter of the tested silica sand is 1.4 to 1.7 mm, which is slightly larger than that of the computed sand. The applied stress is calculated by normalising the platen force by the initial diameter of the agglomerate or the sand grain. A similarity in the response is obtained, in which both the computer simulation and the experimental single particle crushing test results produce a lower peak before the maximum peak strength. After the agglomerate is split at the maximum stress, the platens continue to approach one another with low contact stresses until they find another good contact on the disintegrating agglomerate, to generate another split.
The survival probability of a batch of 20 agglomerates was calculated. The Weibull distribution can be used to describe the variability in tensile strengths of apparently identical test-pieces of a brittle material, in which the survival probability \( s_P \) is a function of normalised stress \( \sigma / \sigma_0 \) given by

\[
P_s = \exp \left[ - \left( \frac{\sigma}{\sigma_0} \right)^m \right] \tag{4.3.1}
\]

where \( \sigma_0 \) is the stress at which \( 1/e \) or 37% of sample survive and \( m \) is the Weibull modulus. McDowell and Bolton (1998) explain that a similar approach can be used on the compressive normalised strength \( F / d^2 \) in grain crushing tests treated as indirect tension tests, where \( F \) is the greatest force that was carried and \( d \) was the initial separation of the platens. Figure 4.3.2 shows that a similar shape of the survival probability curve is obtained when the crushing peak stress is normalised by \( \sigma_0 \), although the silica sand has \( \sigma_0 = 31 \text{ MPa} \) and the simulated agglomerate has \( \sigma_0 = 58 \text{ MPa} \). In addition, both of them give similar values of Weibull modulus of approximately 3. Robertson (2000) showed that the Weibull modulus of a flawed agglomerate depends on the proportion of spheres was removed, or bonds weakened.

### 4.3.3 ASSEMBLY OF MODELLED GRAINS

#### Assembling for modeled grains

For each of the numerical tests reported here, an initial set of “exo-spheres” was first created at a size slightly smaller than the required agglomerates. They were placed at random, but excluding overlaps. Then they were expanded to the required size, and cycled to equilibrium so as to reduce unwanted gaps. During this process shear stiffness and friction were reduced to zero, while normal stiffness was increased 100-fold. A linked list storing the co-ordinates of their centres was then created and the exo-spheres deleted. Randomly rotated aggregates were then created in their place, centred at the co-ordinates in the list as shown in Figure 4.3.3, and the assembly cycled to equilibrium again before commencing the tests. To reduce the likelihood of bonds between balls breaking during this stage, the strengths of the bonds were initially set very high and reduced after a number of cycles. The final shear and normal stiffnesses of the balls of the agglomerates were set to their final values \( (4.0\times10^6 \text{ Nm}^{-1}) \) and their coefficient of friction set to 0.5 (corresponding to a contact friction angle of 26.5°). Finally, bond strengths were fixed and variability was provided in order to achieve the statistical distribution of breakage strength.

#### Mechanical behaviour of assembly

Isotropic compression of a cubical arrangement of 389 agglomerates was begun by slow compression to 20kPa, calculating the equilibrium at each 10kPa increment using a numerical iteration method recommended by the PFC\(^{3D} \) manual and described in detail by Robertson (2000).
Then, the sample was isotropically compressed by 6 smooth stiff walls moving at a slow controlled rate. The voids ratio, calculated by using the solid volume as the total volume of the spheres, was then 2.08, shown as the initial condition.

Figure 4.3.4 shows a comparison of isotropic compression curves between the silica sand and the DEM simulation with a platen approach rate of 1 m/s. The effects of strain rate were investigated by Cheng, et al. (2003). There is a noticeable dynamic effect on the compression behaviour above 1 m/s. The silica sand has a more gentle transition into what we now recognise as clastic compression. One explanation is that real sand particles have a greater variety of asperities, compared with the uniform micro-spheres in the DEM simulation. The opportunities for both elastic compression and crushing at points of contact will be more variable. Similarly, the "normal compression line" in the DEM simulation begins to stiffen below e/e_i of 0.6, in contrast to the real sand. This is also tentatively attributed to the fact that agglomerates only have a limited number of component spheres.

**Necessity of modeled grains**

Figure 4.3.5 shows the e – log p curve for three particulate media having different properties of crushing calculated with 0.05m/sec of walls moving. The thick black line shows the compression result of the crushable assembly of agglomerates with 20% of the balls removed randomly from the regular array, as described earlier. The agglomerates were supposed to have randomness of shape and flaws. The thin black line represents the e – log p curve of the same assembly of agglomerates with the same amount of elementary balls removed but the contact bonds that exist between the balls were non-breakable in this case. The e – log p curve of the breakable agglomerates first deviated from that of the unbreakable ones at 6MPa and started to curve at 17MPa heading to the point known as the yield point. From a stress of 40 MPa onwards, the e – log p plot looks almost linear with of 0.4. The amount of volumetric decrease for the thin black line is significantly small, and the micro mechanism was restricted to the elasticity at contacts and rearrangement of the very rough agglomerates. Comparing the two lines shows that crushability is essential for a realistic representation of plastic deformation with DEM.

The thick grey line of Figure 4.3.5 represents an assembly of agglomerates without removal of any elementary balls from the regular array, although the bonds are crushable. Not only was the initial void ratio much less, there was also an apparent structural effect during the clastic yielding process. The sudden drop in volume at a nearly constant mean stress of 60MPa is due to the uniform crushing nature of these agglomerates without provision of randomness by ball removal, as was seen in the compression of glass beads as reported by Nakata et al (2001). The variability in the crushing strength of agglomerates with no balls removed was low, with a Weibull modulus of 9, compared with that of agglomerates with 20% of balls removed randomly, which had a Weibull modulus of 3. A similar tendency has been observed and discussed for undisturbed aged clay, sedimentary soft rock and cemented soils (e.g. Leroueil and Vaughan, 1990). The structure of materials having a sharp breakdown at yield is considered to be regular due to aging or adhesion processes.

The size distribution of the agglomerates was calculated and shown in Figure 4.3.6. The horizontal axis is the representative size, defined as the 1/3 power of the current solid-volume of each individual agglomerate, while the vertical axis is the percentage of volume reduction. The curves correspond to the particle size distribution curves in real sieving analysis. Initially, the agglomerates were nearly uniform in size. As mean stress increased, the agglomerates became well-distributed in size. It is similar to the evolution of real particle size distribution. The smallest size, however, was restricted by the size of the single elementary sphere.
In order to further understand the significance of the introduction of crushability into the simulation, the constant mean stress triaxial compression shearing tests were calculated for both breakable and unbreakable agglomerate assemblies after they were normally - compressed to various pressures, i.e. the thick and thin black lines respectively in Figure 4.3.5. Figure 4.3.7 shows the results for the breakable agglomerate assembly compressed by rigid walls for: (a) the stress-strain curves and (b) the volumetric and deviator strain curves. The volumetric behaviour with initial confining pressures of 1 and 5MPa were dilative. As the initial confining pressure increased, the drained behaviour changed from dilative to contractive. In the cases with initial confining pressure of 20 and 40MPa, the volumetric strain reached 15% contractively. The constant volumetric strain condition at the final stage of the test appeared in the case of 1 – 10 MPa of mean stress. The results for the unbreakable agglomerate assembly are shown in Figure 4.3.8. Shearing at all levels of initial confining pressure produced volume changes that were dilative although the degree of dilation became slightly weaker as the initial confining pressure increased.

Applications of modelled grains
(1) Understanding of Critical State
The whole series of drained and undrained test paths is shown in Figure 4.3.9, together with indicative arrows if the final state of the simulation was continuing to change when the computation was terminated. There is some ambiguity in the corresponding location of a critical state line on the e versus log $p'$ plot. In particular, the drained test with $\sigma'_3 = 20\text{MPa}$ was continuing to reduce in volume as bonds continued to suggest that the dissipation function used in Cam Clay would be improved if grain damage and grain rearrangement were recognised as distinct micro-mechanisms.
(2) Understanding of plastic deformation and crushing
The yield point was determined in the conventional way as a change in the slope of a stress-strain curve for an over-consolidated DEM element. The element (with $e_i = 2.08$) was first loaded to 40 MPa and then unloaded to 20 MPa, giving an over-consolidation ratio defined with respect to $p'$ of two ($n = 2$) before stress-path tests were simulated. Fig. 4.3.10(a) shows the corresponding yield points of all stress-path directions in q-$p'$ space from the results of the stress-path shearing tests. The amount of bond-breakage could be quantified by the percentage of broken-bonds (pbb) counted from the beginning of shearing in each stress path. The numerical values of the pbb in a contour representation are shown in Fig. 4.3.10(b). The yield points obtained from the change-of-slope method (Fig. 4.3.10(a)) can be approximated by the four-percent broken-bond contour (pbb = 4%). It is clearly seen that bond breakage occurred before gross plastic yielding could be detected in the stress-strain response. It is therefore clear that a significant proportion of bonds are broken as the stress state moves “inside” the observed yield surface. Significant rearrangement (corresponding to macroscopic yielding) only occurs at about 4% pbb.

Plastic deformation was calculated from the measured total macroscopic strain of the element and the derived elastic strain using $\kappa = 0.04$ but assuming the elastic deviator strain to be negligible. The plastic strain increments were then plotted in Fig. 4.4.10(c). Both of them showed that the plastic flow followed a non-associated flow rule rather than the normality rule, similar to real soil.

4.3.4 CONCLUSION
The usefulness of Distinct Element Method in modelling the behaviour of crushable soil was presented. Numerical grains were made by bonding elementary spheres in “crystallographic” arrays, and by giving each sphere an existence probability of 0.8. The
bonding model which was adopted in the contact points between the spheres to limit the total normal and shear forces. Elementary tests, which were conventionally conducted in geotechnical engineering, on a cubical sample made of 389 grains were simulated. The behaviours of isotropic compression and "drained" triaxial compression under constant mean effective stress showed a reasonable tendency qualitatively. It indicated the use of the modelled grains to be justified in further geotechnical engineering applications.

REFERENCE


4.4 MODELING OF CAPILLARY FORCE

4.4.1 INTRODUCTION

In unsaturated soil, soil water exists as meniscus at contact points between particles. According to the meniscus, pressure difference is induced between pore air pressure and pore water pressure that is called as suction. Suction causes intergranular adhesive force between particles perpendicular to the contact plane as shown in Figure 4.4.1, and it has influence on the complicated behavior of unsaturated soil.

To study the behavior of unsaturated soil, many triaxial tests have been carried out. Based on the triaxial test results, constitutive models have been presented, but some fundamental characteristics in unsaturated soil are still not confirmed. For the compressibility of unsaturated soils, Alonso et al. 1990 proposed one equation in their constitutive model, in which the compressibility index is treated as variable for change of suction. But there have been reported that the compressibility index is treated as a constant value regardless of suction value if the additional induced confining pressure by suction is accounted for total confining pressure (Karube et al. 1986). About the strength property, Fredlund et al. 1978 proposed one equation to represent shear strength for unsaturated soil as follows.

\[
\sigma_f = c_{\text{sat}} + (\sigma - u_a)\tan \varphi_{\text{sat}} + (u_s - u_w) \tan \varphi \quad (4.4.1)
\]

where \(\sigma_f\) : shear stress at failure on the failure plane , \(\sigma\) : normal total stress at failure on the failure plane , \(c_{\text{sat}}\) : cohesion under saturated state, \(\varphi_{\text{sat}}\) : internal friction angle under saturated state, \(\varphi\) : parameter concerning to increase of shear strength with suction increase and \(u_a, u_w\): pore air and water pressure respectively.

In this equation, the internal friction angle is treated as a constant value from saturated state to unsaturated state. But there have been reported a triaxial test result for unsaturated soil under constant suction, in which the internal friction angle increases with the increase of applied suction (Karube et al. 1986). The reason why these different views are proposed is because there are some limitation and problems in the triaxial test for unsaturated soil.

In many cases, the pressure plate method is used in triaxial test for unsaturated soil, in which ceramic disk is used instead of the porous stone, to apply air pressure to specimen. The ceramic disk has own air entry value that limits the maximum applied air pressure, and it leads to the limitation of suction condition. Further, the volume change of the specimen should be measured separately from measuring displacement of the drainage from specimen. According to this condition, the double cell method is used in many cases. But in the double cell method, the volume of the inner cell will change for the lateral pressure applied. We must correct the measurement value of the volume change of specimen for the lateral pressure change, and the obtained results contain some errors. These limitation and problem have influence on the accuracy of the triaxial test for unsaturated soil and the comprehension for behavior of unsaturated soil.

We will not encounter in these limitation and problem mentioned above in simulation with DEM analysis. When we simulate true triaxial test for granular material with adding the intergranular adhesive force, we are able to apply the arbitrary value of the intergranular adhesive force, which corresponds to the applied suction in the triaxial test, and to know the volume of the specimen clearly.

In this study, by the distinct element method analysis in three-dimensional state, simulations of the true triaxial test for spherical granular material is carried out. In this analysis, the influence of meniscus water, which is mainly cause of the complicated behavior of unsaturated soil, is expressed by introducing a constant intergranular adhesive force that acts perpendicular to the tangential plane at contact point. The influences of the intergranular adhesive force on the failure criterion and shear deformation are examined to clear mechanical characteristics of unsaturated soil and the other granular materials with adhesion.

4.4.2 FAILURE CRITERIA FOR SOIL

There have been presented many failure criteria for soil. In this chapter, the failure criteria, which concern to our study, are briefly explained

Mohr-Coulomb failure criterion is widely used in soil mechanics, and it has a shape of deformed hexagonal on the \(\sigma - \varphi\) plane as shown in Figure 4.4.2.

Figure 4.4.3 shows "Spatially Mobilized Plane (SMP)", the direction of which is defined based on the principal values of stress tensor. Based on this plane, Matsuoka...
& Nakai 1974 proposed a failure criterion as follows. The normal and tangential components of the principal stress vector in principal stress space to the SMP are given as follows.

\[
\sigma_{\text{SMP}} = \sigma_1 a_1^2 + \sigma_2 a_2^2 + \sigma_3 a_3^2 = \frac{3I_1}{I_2} \quad (4.4.2)
\]

\[
\tau_{\text{SMP}} = \sqrt{(\sigma_1 - \sigma_2)a_1^2a_2^2 + (\sigma_2 - \sigma_3)a_2^2a_3^2 + (\sigma_3 - \sigma_1)a_3^2a_1^2}
\]

\[
= \sqrt{I_1I_2 - 9I_3^2} 
\]

Where \(a_1, a_2, \) and \(a_3\) are the direction cosines for the SMP given as follows.

\[
a_i = \sqrt{\frac{I_i}{\sigma_i I_2}} \quad (i = 1, 2, 3) \quad (4.4.4)
\]

Here \(I_1, I_2, \) and \(I_3\) are the invariants of principal stress defined as

\[
I_1 = \sigma_1 + \sigma_2 + \sigma_3 \quad , \quad I_2 = \sigma_1\sigma_2 + \sigma_2\sigma_3 + \sigma_3\sigma_1 \quad , \quad I_3 = \sigma_1\sigma_2\sigma_3 \quad .
\]

The next equation is obtained, by taking the condition that the ratio of the normal component to the shear component becomes a constant value as the SMP failure criterion.

\[
\frac{\tau_{\text{SMP}}}{\sigma_{\text{SMP}}} = \sqrt{\frac{I_1I_2 - 9I_3^2}{9I_1^2}} = \text{const}
\]

\[
= \frac{2}{3} \sqrt{\frac{\sigma_1 - \sigma_2}{2\sqrt{\sigma_1\sigma_2}}} + \frac{\sigma_2 - \sigma_3}{2\sqrt{\sigma_2\sigma_3}} + \frac{\sigma_3 - \sigma_1}{2\sqrt{\sigma_3\sigma_1}} \quad (4.4.5)
\]

And eliminating the effect of confining pressure from the above equation derives the next equation.

\[
\frac{I_1}{I_3} = \text{const} \quad (4.4.6)
\]

Figure 4.4.4 shows the SMP failure criterion of Equation (4.4.6) and the Mohr-Coulomb failure criterion plotted on the \(\pi\) plane. The SMP failure criterion shows the same shear strength at the triaxial compression and the triaxial extension stress state as those shown by the Mohr-Coulomb failure criterion, but in the other conditions, it shows stronger shear strength.Lade & Duncan 1975 carried out true triaxial tests for sand specimens under different stress paths on the \(\pi\) plane. Based on the obtained true triaxial test results, they proposed the failure criterion shown as the next equation

\[
\frac{I_1}{I_3} = k_3 \quad (4.4.7)
\]

Where \(k_3\) is a constant that represents the shear failure state.

Figure 4.4.5 shows the Lade failure criterion of
Equation (4.4.7) plotted on the $\pi$ plane. As shown in this figure, the Lade failure criterion shows slightly different shape for the different internal friction angles. Figure 4.4.6 compares the Lade failure criterion with the Mohr-Coulomb failure criterion on the condition that they have the same internal friction angle at the triaxial stress state. From this figure, it is understood that the Lade failure criterion has bigger internal friction angle than the Mohr-Coulomb failure criterion at the triaxial extension stress state.

4.4.3 DEM ANALYSIS AND ANALYTICAL CONDITION

Outline of DEM analysis with intergranular adhesive force

The distinct element method (DEM) is one of the discontinuous corpora analysis method proposed by Cundall 1971. Unlike continuum analysis of the finite element method or the boundary element method, it is suitable for analyzing the dynamic behavior of the granular material. In the DEM analysis, simple dynamic models (they are generally the Voigt model and Coulomb’s friction rule) are introduced for normal and tangential directions to the contact plane at contact points and contacting surfaces between the particles with the assumption that the particles are rigid. The independent equations of motion for every element are solved forwardly in the time domain, and the interactions between particles and the deformation of particle aggregates are traced. This method has the merit that the necessary output data are easily obtained, such as stress, strain, and rotation angle of some particles, and the setting of boundary conditions. In this study, we carried out the analysis with the distinct element analysis system “PFC3D” programmed by Itasca Co, Ltd.

In the two dimensional analysis, the effect of meniscus water observed in unsaturated soil is expressed by introducing an intergranular adhesive force between particles as follows. The intergranular force acting between contacting particle i and j is denoted as $P_{ij}$. The x and y direction components, and the moment component of the resultant force of the intergranular adhesive force at time t are given by the following equations considering that the direction of $P_{ij}$ is normal for the line direction of the particle tangent plane.

$$[F_x]_t = \sum_j P_{ij} \cos \alpha_{ij} \quad (4.4.8)$$

$$[F_y]_t = \sum_j P_{ij} \sin \alpha_{ij} \quad (4.4.9)$$

$$[M]^t = 0 \quad (4.4.10)$$

Where, $[F_x]_t, [F_y]_t, [M]^t$ are the x and y direction components, and the moment component of the resultant force of the intergranular adhesive force and $\alpha_{ij}$ is the angle between the normal direction of the contact plane and the x-axis.

It is possible to introduce an intergranular adhesive force by deducting these components from each component of the total intergranular force except for the intergranular adhesive force. By integrating these equations of motion for each particle by the Euler method with respect to time, the analysis was carried out. Consequently, the solution becomes stabilized conditionally on the integral time increment. In the three dimensional analysis, the similar procedure is applied.
Cundall 1971 proposed the following equation for the integral time increment.

\[ \Delta t < \Delta t_c = 2 \sqrt{\frac{m}{k}} \quad (4.4.11) \]

Where, \( k \) is mass of the disk particle, and \( m \) is the spring constant.

It has been found experientially that sufficient stability and accuracy can be ensured in the quasistatic problem at about 1/10\( \Delta t_c \), though equation (4.4.11) is deduced from the equation of motion for a single-degree-of-freedom system. But taking this equation as a standard, the integral time increment must be decided by trial and error. In this study, \( \Delta t = 8/10 \Delta t_c \) is used. The parameters and the material properties necessary for the analysis are listed in Table 4.4.1.

### Analytical condition

A rectangle specimen of 5 meters height, and 2 meters width and deep was used for the analytical model as shown in Figure 4.4.7. The particles, whose diameters ranges from 0.05 m to 0.10 m, are placed randomly inside the specimen, but the numbers of each particle are controlled in condition that they keep the Gaussian distribution in the frequency distribution of the particle diameters. Totally 5438 particles are placed inside the specimen, the void ratio of which is about 0.4. The six sides of the rectangle specimen are surrounded by the rigid wall elements that correspond to the loading platens.

In this study, firstly, without the intergranular adhesive force, the specimen was compressed isotropically under confining pressures of 500 and 1000 kPa. Then, the intergranular adhesive force of 5000 N or 10000 N was introduced between particle contact points. The same specimens are used for different stress paths on the \( \pi \) plane, and the void ratio of the specimen and the state of particle distribution before the shear process are the same state for the each series of different stress paths under constant mean principal stresses on the \( \pi \) plane. Afterwards, the shear process of the true triaxial test was simulated under the constant mean principal stress. When the shear process of the true triaxial test was simulated, the upper and bottom wall elements were moved perpendicularly at a constant rate of 10cm/s in order that the maximum principal stress applied for the height direction. And the other pairs of lateral wall elements were controlled to keep the decided stress path and constant mean principal stress condition. Figure 8 shows the stress paths on the \( \pi \) plane under confining pressures of 500 and 1000 kPa. In one stress path, one kind of Lode parameter \( \theta \) was kept constant at 60, 75, 90, 105 and 120 degrees.

### 4.4.4 TEST RESULTS AND DISCUSSIONS

**Effects of intergranular adhesive force on failure**
Figures 4.4.9 and 10 show the stress-strain relations for triaxial stress state and triaxial extension state under confining pressure of 1000 kPa. In these results, the principal stress difference showed bigger peak value with the increase of the intergranular adhesive force, and then decreased. And the more expansive behavior were observed with the increase of the intergranular adhesive force. These results are similar with that observed in the triaxial compression test for unsaturated clay specimen under different constant suctions (Karube et al. 1986). The intergranular adhesive force resists for the slippage at contact points between particles, and affects on these observed behaviors. The increase of shear strength is deduced, but the increase of volume expansion is not deduced simply from the effect of the intergranular force.

Figure 4.4.11 shows relation between maximum principal stress differences and means principal stress. The dots show simulation results and the solid lines show the failure lines for each intergranular adhesive force. These results, we find that the increase of intergranular force has influence not only on the adhesion but also on the

influence of the suction was not clear. But based on these results, we are able to state that the increase of the intergranular adhesive force causes the increase of the internal friction angle.

Table 4.4.2 Adhesion and internal friction angle obtained

<table>
<thead>
<tr>
<th>Adhesion (N)</th>
<th>c (kPa)</th>
<th>φ (degrees)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>4.9</td>
<td>20.37</td>
</tr>
<tr>
<td>5000</td>
<td>-31</td>
<td>40.70</td>
</tr>
<tr>
<td>10000</td>
<td>-140</td>
<td>42.18</td>
</tr>
</tbody>
</table>

Figure 4.4.10 Relation between maximum principal stress differences and means principal stress

Figure 4.4.11 Stress-strain relation for triaxial extension stress state under different intergranular adhesive forces
Figure 4.4.12 Maximum shear stress states on the $\mathbf{K}$ plane. In this figure, the solid lines shows the Mises failure criterion, and the broken line and the one dotted lines show the Lade and the Mohr-Coulomb failure criterion, which correspond to the internal friction angles at triaxial stress state, respectively.

Figure 4.4.13 shows the normalized data shown in Figure 4.4.10 by changing the scale that the results of 5000 N and 10000 N of internal adhesive forces have the same $\mathbf{M}_z$ intersect as that for the result of no internal adhesive force. In this figure, The solid line and the one dot line show the Mises and the Mohr-Coulomb failure criterion, and the broken line and the two kinds of two dotted line show the Lade failure criterion for different internal friction angle. From these results, we find that the Lade failure criterion is able to explain the failure stress state, regardless of the value of the intergranular adhesive force.

**Effects of intergranular adhesive force on residual stress state and shear deformation**

Figures 4.4.14 and 15 show the residual stress states for the case of no intergranular adhesive force and 10000 N of intergranular adhesive forces. As shown in Figures 4.4.9 and 10, the residual stress state is not
clear in the stress-strain relations, but we decided it as the stress state when the axial strain is 20%. In these figures, the solid line, the broken line and the dotted line show the Mises, the SMP and the Mohr-Coulomb failure criterion respectively. From this figure, we find that the SMP failure criterion explains the residual stress state well. This result corresponds to the result of true triaxial test for normally consolidated clay specimen (Shibata & Karube 1965), in which the failure stress states are plotted on the plane as a circumscribed curve for the Mohr-Coulomb failure criterion in the similar way as the SMP failure criterion does as shown in Figure 4.

Figure 4.4.16 shows the counters of equivalent shear strain on the plane. From the origin to outside direction, the each curve shows counter of shear strain from 0.003 to 0.01 by 0.01 division respectively. The dotted curve and the solid curve show the result of no intergranular adhesive force and 10000 N of intergranular adhesive forces respectively. In the case of no intergranular adhesive force, the solid curves are near to concentric shape, but in the case of 10000 N of intergranular adhesive forces, the dotted curves are deformed from the concentric shape.

Figure 4.4.17 compares the stress points at same shear strain near to the failure state with the Lade failure criterion. From this figure, we find that the stress points distribute around the Lade failure criterion. From the results shown in Figures 4.4.16 and 17, we should conclude that the Lade failure criterion explains the counters of shear deformation, and dominate the shear deformation of expansive granular materials.

4.4.5 CONCLUSIONS

By the distinct element method analysis in three-dimensional state, simulations of the true triaxial test for spherical granular material was carried out. In this analysis, the influence of meniscus water, which is mainly cause of the complicated behavior of unsaturated soil, is expressed by introducing a constant intergranular adhesive force that acts perpendicular to the tangential plane at contact point. The influences of the intergranular adhesive force on the failure criterion and shear deformation are examined. The obtained results are summarized as follows.

The internal friction angle and the adhesion for triaxial stress state increased with the intergranular adhesive force. This result corresponds to the triaxial test results obtained for unsaturated soil, and shows the effectiveness of introducing the intergranular adhesive force for DEM analysis to study the mechanism of unsaturated soil and the other granular materials with cohesion.

The Lade failure criterion on the plane explained well the failure stress state regardless of the intergranular adhesive force. This result means that the
Lade failure criterion is able to use the failure criterion for unsaturated soil and the other granular materials with cohesion.

The residual stress points on the $\Box$ plane distribute around the SMP failure criterion. This result means that the SMP failure criterion is able to use the contractive material like normally consolidated clay.

The counters of shear strain show the similar shape with the Lade failure criterion at near to failure state. This result shows that the Lade failure criterion should dominate the shear deformation of expansive granular materials with cohesion.

References


4.5 TWO-Scale (Global-local) Modeling for Granular Media

4.5.1 Introduction

Granular media such as powders and sands are regarded as composite materials that reveal fine scale heterogeneities with the friction and contact. Common to the mathematical modeling is the recognition that the local region is occupied by discrete particles, while the region is identified with a material point in the overall structure. Since the materials reveal such two-scale nature, the characterization of the mechanical behavior of granular materials intrinsically involves two distinct scales, namely micro and macro-scales. In this section, we propose a numerical method of two-scale (global-local) analyses for granular media with reference to Terada and Kikuchi (2001), which presents the general procedure to have the two-scale boundary value problem (BVP) within the framework of the mathematical homogenization theory. The mathematical theory of homogenization for heterogeneous media with periodic microstructures enables us to realize the consistent two-scale modeling, which entails both micro- and macro-scales together with variational statements; see, e.g., Sanchez-Palencia (1980); Lions (1981); Benssousan, et. al. (1978). The problem can be formulated in terms of two distinct scales; macro- and micro-scales. The former scale defines a macroscopic (global) structure composed of granular assemblies, each of which corresponds to a microstructure or equivalently a representative volume element (RVE) given in the latter scale. The macroscopic field variables are simply obtained as the volume average of the corresponding microscopic ones over the RVE and meet a quasi-static equilibrium of the overall structure. On the other hand, the particulate nature with the cohesive-frictional contact behavior is given to the RVE in a micro-scale. The RVE is assumed to be periodic and is often re-phrased as a unit cell. Then, the derived two-scale boundary value problem allows us to analyze the micro-scale behavior of unit cells by a granular element method (GEM; Kishino (1989)), in which spring and cohesive-frictional devices connect rigid particles with each other, while the macroscopic problem is solved by the conventional continuum-based FEM. After formulating the two-scale boundary value problem, we construct the numerical algorithm. Moreover, we apply the developed two-scale numerical model to the simple two-scale simulations for granular materials. The intimate relationship between the microscopic deformation mechanisms in unit cells and the macroscopic mechanical behavior is illustrated in a numerical manner. Then, we discuss the applicability and feasibility of the proposed method.

4.5.2 Two-Scale Modeling for Granular Media

We consider the quasi-static boundary value problem of a granular body shown in Fig. 1(a). The body is regarded as an assembly of periodic arrangements of basic microstructural elements (called unit cells), which are composed of a random distribution of elastic particles and voids (Fig. 1(b)). It is assumed that the size of a unit cell is small enough to the overall structure and is represented by a normalized parameter \( \varepsilon \). We also assume that the problem is 2-dimensional and that the particles are ideally circular disks.

![Figure 4.5.1](https://example.com/figure.png)

**Variational formulation of friction-contact problem**

Let \( \Omega^c \) be an open domain of the granular body, and be divided into \( \Omega^c_\ell \), \( \Omega^c_L \), and \( C^e \) as \( \Omega^c = \Omega^c_\ell \cup \Omega^c_L \cup C^e \), where \( \Omega^c_\ell \) is an open domain of particles, \( \Omega^c_L \) is an open domain of voids and \( C^e \) is the totality of the internal surfaces associated with contact and friction. We also define the partial open domain \( \Omega^c_L \) by excluding \( C^e \) from \( \Omega^c \), i.e. \( \Omega^c_L = \Omega^c \setminus C = \Omega^c_\ell \cup \Omega^c_L \). Then, this problem is fully described by the equilibrium problem in \( \Omega^c_\ell \) and friction and contact conditions on \( C^e \).

The equilibrium equation for the stress \( \sigma^e(x) \) in \( \Omega^c_\ell \) and boundary conditions on \( \partial \Omega^c_\ell \), which is an external surface of this body, are respectively given by

\[
\text{div} \; \sigma^e(x) + b^\ell(x) = 0 \quad \text{in} \; \Omega^c_\ell, 
\]

\[
u^\ell = 0 \quad \text{on} \; \partial \Omega^c_\ell, \quad \text{and} \; \sigma^e n = t \quad \text{on} \; \partial \Omega^c \]

where \( b^\ell(x) \) is the body force, \( t \) is the traction vector specified on \( \partial \Omega^c \) with the outward unit normal \( n \); \( u^\ell \) is the displacement. Here, and in the subsequent sections, we indicate the dependency on the microscopic heterogeneities by a superscript \( \varepsilon \) on each variable. It is also assumed that individual particles and voids reveal elasticity and has the following constitutive equation:

\[
\sigma^e(x) = D^e(x) \varepsilon^e(x),
\]
where $\epsilon^e(x)$ is an infinitesimal strain and $D^e(x)$ the elasticity tensor, which is symmetric and positive definite (it is 0 in the voids if the body is fully dry). The strain is related to the displacement by the following relationship as usual:

$$\epsilon^e(x) = \nabla^{(s)}u^e,$$

where $\nabla^{(s)}$ is a gradient operator which produces a symmetric part of an arbitrary second-order tensor.

In order to provide the complete set of governing equations, we here define the friction and contact conditions on $C^e$. Figure 4.5.1(c) shows the illustration of the friction and contact conditions on a particle $a$, on which the outward unit normal $n^e$ and the unit tangential vector $t^e$ are defined so that $(n^C, t^C)$ can be a set of base vectors for the right-hand local coordinate system. Then, the displacement vector $u^e$ and the stress vector $T^e$ on $C^e$ are decomposed respectively into their normal and tangential components as follows:

$$u^e = \left\{u^e_n, u^e_t\right\}^T$$

$$T^e = \left\{T^e_n, T^e_t\right\}^T$$

Using these components, we have the contact condition (4.5.5) and (4.5.6) for contact and friction conditions (4.5.1)-(4.5.4) in particles, is completely described by the equilibrium equations (4.5.1)-(4.5.4) in $\Omega^e$. Figure 4.5.2 Decomposition to micro- and macro-space.

Two-scale boundary value problem

It has been demonstrated in Terada and Kikuchi (2001) that the theory of two-scale convergence of Allaire (1992) can be utilized in the derivation of the two-scale boundary value problem for a heterogeneous solid with periodic microstructures.

A distinguished idea of the mathematical homogenization theory is to introduce two distinct scales: macro- and micro-scaling. $x$ and $y$, the latter of which is related to the former $y=x/\epsilon$. Due to the introduction of these two spatial scales, the domain $\Omega^e$ composed of particles and voids is divided into $\Omega$ measured by the macroscopic variable $x$ and $Y^e = Y \setminus \Omega$ measured by the microscopic one $x$ as follows (see Fig. 4.5.2):

$$\Omega^e = \Omega \times Y^e = \left\{ (x, y) \big| x \in \Omega \subset \mathbb{R}^3, y = x/\epsilon \in Y^e \subset \mathbb{R}^3 \right\}$$

where $\Omega$ is a microscopic domain and $C$ is the contact region. With this decomposition, all the field variables with superscript $\epsilon$ are re-defined as functions of two scale variables $(x, y)$:

$$u^e(x) = u(x, y), \quad b^e(x) = b(x, y), \quad \epsilon^e(x) = \epsilon(x, y), \quad \sigma^e(x) = \sigma(x, y), \quad D^e(x) = D(x, y)$$

each of which is periodic with respect to $y$, i.e. $Y$-periodic.

In this particular situation for granular media, the similar argument would hold for the variational inequality (4.5.7) and the following formula can be obtained as a limit of the appropriate convergence study:

$$\int_{\Omega} \nabla \cdot (\epsilon(x) - \epsilon^0 - u) \cdot \nabla \epsilon(x) \ dx + \int_{\Omega} \nabla \cdot (\epsilon^0 - u) \cdot \nabla \epsilon^0 \ dx$$

$$+ \int_{\Omega} \nabla \cdot (\epsilon^0 - u) \cdot \nabla \epsilon(x) \ dx + \int_{\Omega} \nabla \cdot (\epsilon^0 - u^e) \cdot \nabla \epsilon(x) \ dx$$

$$- \int_{\Omega} \nabla \cdot (\epsilon^0 - u^e) \ dx \geq 0, \quad \forall \nu^0 \in \nu, \forall \nu^1 \in K^e,$$

where $\nu^0 \in \nu, \forall \nu^1 \in K^e$. In which $H^1(\Omega^e)$ is the Sobolev space of order one.
where \( \langle \cdot \rangle \) indicates the volume average over the unit cell domain \( Y \). Here, \( u^0 \) and \( v^0 \) are independent of the microscopic heterogeneities and can be chosen from the following admissible functional space \( V \) on \( \Omega \):

\[
V = \{ v^0(x); v^0 \in H^1(\Omega) \cap V; v^0 = 0 \text{ on } \partial \Omega \},
\]

whose measure is the macroscopic variable \( x \). On the other hand, the microscopic displacement (trial function) \( u^l(x,y) \) and its variation (test function) \( v^l(x,y) \) are \( Y \)-periodic and regarded as elements of the subset \( K_{Y_c} \) of a linear space \( V_{Y_c} \), which are respectively given by

\[
V_{Y_c} = \{ v^l(x,y); v^l \in H^1(\Omega \times Y_c) \cap Y; \text{ } \text{ } \text{ } \text{ } Y \text{-periodic} \},
\]

\[
K_{Y_c} = \{ v^l(x,y); v^l \in V_{Y_c}; \| v^l \| \geq 0 \text{ on } C \}.
\]

In inequality (4.5.11), the test function \( v^l \) can be chosen as \( v^l = u^l \), while \( v^0 \) can be chosen as \( v^0 = u^0 + \alpha w^0 \) (because \( V \) is a linear space), where \( w^0 \) is an arbitrary function in \( V \) and \( \alpha \) is an arbitrary real number. Then, inequality (4.5.11) yields the following equality:

\[
\int_{\Omega} \nabla_x (w^0) : \left\langle D \left( \nabla_x (u^0) + \nabla_y (u^l) \right) \right\rangle \right] dx = \int_{\Omega} \langle b \rangle : w^0 dx + \int_{\partial \Omega} t \cdot w^0 d\Gamma,
\]

(4.5.12)

This equation of virtual work is solved for the average displacement \( u^0 \) of overall structure, and involves the effect of microstructures in \( \nabla_y (u^l) \) of its left-hand side.

On the other hand, in inequality (11), \( v^0 \) can be set to \( v^0 = u^0 \) and \( v^l \) to \( v^l = u^l + \alpha w^l \) with variation \( w^l \in K_{Y_c} \) and a real number \( \alpha \geq 0 \) \( (\alpha \) is always positive since the space \( K_{Y_c} \) is a convex cone in the particular case). Then the variational inequality for \( u^l \) in the unit cell yields

\[
\int_{Y_c} \nabla_y (w^l) : D : \nabla_y (u^l) dy + \int_{Y_c} \mu \| T_e (u^l) \| \| w^l \| ds - \int_{Y_c} \mu \| T_e (u^l) \| \| w^l \| d\Gamma \geq -\left( \int_{Y_c} \nabla_y (w^l) : D : \nabla_y (u^l) \right) \right] dx \left( \left[ u^l \right] \right) \forall w^l \in K_{Y_c},
\]

(4.5.13)

where \( \nabla_y (u^l) \) plays a role of the constant excitation corresponding to the macroscopic behavior. Although the solution of the variational inequality (4.5.13) is not unique on \( K_{Y_c} \), but can be unique on the restricted convex cone \( K_{Y_c} \), which is defined as (Sanchez-Palencia (1980)):

\[
K_{Y_c} = \{ u^l(x,y); u^l \in K_{Y_c}; \| u^l \| = 0 \}.
\]

The average behavior of the overall structure can be characterized by the solution of (4.5.12) under the influence of the microstructure whose mechanical behavior is characterized by (4.5.13). Consequently, the above macroscopic problem has a solution as long as the microscopic problem has a solution, which is described in the next subsection. These micro- and macroscopic simultaneous equations govern a two-scale boundary value problem for a granular medium.

### 4.5.3 Solution Scheme of Global-Local Computations

The macroscopic equilibrium equation (4.5.12) can be re-written as

\[
\int_{\Omega} \nabla_x (w^0) : \Sigma dx = \int_{\Omega} \langle b \rangle : w^0 dx + \int_{\partial \Omega} t \cdot w^0 d\Gamma, \quad \forall w^0 \in V
\]

(4.5.14)

where the macroscopic stress is given by

\[
\Sigma = \left\langle D \left( \nabla_x (u^0) + \nabla_y (u^l) \right) \right\rangle.
\]

(4.5.15)

On the other hand, the microscopic equation (4.5.13) governs the conventional friction-contact problem, but is defined in \( Y \) and excited by the macroscopic deformation. We note that the equations in both scales are completely coupled, but can be solved independently by a sequential solution scheme in each loading step. Therefore, the microscopic problem is solved by the analysis codes that can handle the friction-contact problem for elasticity, while the macroscopic one is by a conventional finite element method analysis code with slight modification.

Now, let us assume that a simple physical model that is composed of rigid particles (circular disks in a plane specimen), springs, frictional slides and tension-cutoff devices can replace the microstructure; see Fig. 4.5.3. That is, the stiffness or deformability of particles in \( Y \) is replaced by the stiffness of springs and the friction-contact and cohesive condition on \( C \) by frictional and tension-cutoff devices respectively, both of which connect particles with each other. This type of models is readily solved by one of them; e.g., the granular element method (GEM) (Kishino, 1989).

In the formulation of GEM, the unit normal and tangential vectors, the degrees of freedom and the contact forces applied from adjacent particles on \( C \) are defined as shown in Fig. 2. In spite of evaluating the stress for deformable particles, the macroscopic stress is approximated with energy arguments as

\[
\Sigma(x) \approx \frac{1}{|Y|} \sum T^E \cdot y^E
\]

(4.5.16)
Figure 4.5.3 Illustration of concept of granular element method

where $|Y|$ is the initial volume of a unit cell, $T^E$ is the traction force applied to the boundary particles from exterior particles and $y^E$ is the initial position of the contact point. Though the microscopic stress cannot be defined for rigid particles, the macroscopic stress is expected to be that for a material point of the homogenized continuum. In actual computations, the two-scale BVP is solved in an incremental manner for given loading. In each loading step, the microscopic self-equilibrated state is obtained to evaluate the macroscopic stress by (4.5.16) for macroscopic equilibrium (4.5.14). It should be noted that the role of microscopic analysis by GEM is the constitutive relation for a macroscopic material point. A concept of two-scale analysis is shown in Fig. 4.5.4. One can refer to the more details of GEM and the global-local numerical algorithm are found in the literatures (Kishino (1989) and Kaneko et al., (2002)).

Figure 4.5.4 Concept of two-scale analysis method

4.5.4 REPRESENTATIVE NUMERICAL EXAMPLES

Bi-axial compression tests for non-cohesive granular media

The finite element model of the macroscopic overall structure under consideration is shown in Fig. 4.5.5(a) together with boundary conditions. Here, the displacements on the top and bottom surfaces of length $L$ are fixed. The displacement at the top surface is controlled to compress the model for various values of confining pressure; $p^0 = 0.2$, $0.3$ and $0.4$ MPa. On the other hand, the unit cell model for the micro-scale granular element analysis is shown in Fig. 4.5.5(b), which has about 200 particles. Physical parameters are given as follows: the normal spring constant $50$ kN/m, the tangential one $35$ kN/m, the friction coefficient 0.466.

Before providing the results, we define several physical quantities measured in the following numerical experiments. First of all, the apparent stress and strain for specimens are defined as macroscopic quantities just as those defined in experiments for soils and sands.

Figure 4.5.5 Macro- and microscopic analysis model

For example, the axial stress is an apparent quantity, which is evaluated as the nominal stress $\sigma_{\text{axial}} = P/L$ with $P$ being the reaction force at the bottom of the specimen. Thus, the deviator stress is defined as $\sigma_{\text{dev}} = \sigma_{\text{axial}} - p^0$. The axial strain is also a macroscopic and apparent quantity defined as $\epsilon_{\text{axial}} = \Delta H/H_0$ where $\Delta H$ is the height change of a specimen with initial height $H_0$. In view of geotechnical applications, apparent volumetric change called dilatancy is worth to be identified with the volumetric stain $\epsilon_{\text{vol}} = \Delta V/V_0 - 1$ where $V_0 = L H_0$ is the initial volume and $V$, which is calculated by adding the volume of all elements, is the one after deformation.

Figure 4.5.6 Stress-strain and dilatancy curves
Figure 4.5.6 shows the relationship between the apparent (macroscopic) deviator stress, $\sigma_{\text{div}}$, and the axial strain, $\varepsilon_{\text{axial}}$, for various values of confining pressure. As can be seen from this figure, the response is almost linear at the very beginning of loading, and gradually reveals nonlinearity for all the cases. The figure also presents the relationship between the dilatancy characteristics of the specimen and the axial strain. We can see that the compressive loading makes the specimen dilate at the early stage of loading and reach the peak of the curve. In addition, three different stress-strain curves illustrate the pressure dependent behavior, which is known to be peculiar to granular materials. These results seem similar to the ones observed in actual experiments such as tri-axial tests for sands. Note, however, that these measured quantities are apparent ones as mentioned in the above and are not necessarily the same as actual field variables.

The process of the macroscopic deformation under confining pressure 0.3MPa is presented in Fig. 7, in which the slack-type deformation is well demonstrated as can be expected. Also, Figure 8 shows the distributions of the volumetric strain $\varepsilon_{\text{vol}}$. Although the dilatancy observed in Fig. 6 is an apparent one for the overall structure, the characteristics recognized from Fig. 8 show that the material itself reveals dilatancy around the center of the specimen when the axial strain reaches 2.0%. In the stage of 2.4% axial strain, material points around the center of the specimen dilate about 0.5% though the overall structure is compressed in the axial direction. This implies that the internal structure of the granular material, i.e., the microstructure, increases its volume. Such behavior of unit cells results from the motion of particles with frictional contact as can be seen later. Thus, the developed two-scale model can reflect the particulate nature in unit cells and reproduce the typical macroscopic deformation characteristics such as the pressure dependency and the dilatancy.

It is, however, difficult to estimate the overall strength of the specimen by the analysis. In this context, Figure 4.5.9 shows the distributions of the semi-norm of the deviator strain under bi-axis compression. As can be seen from the figure, the shear-dominant deformation gradually concentrates around the center of the specimen and eventually appears to exhibit the preferable orientation of concentration. Although this is a typical phenomenon observed in compression tests, our global-local computation cannot simulate the formation of a macroscopic slip surface, which leads to overall collapse.
Figure 4.5.9 Distribution of the norm of deviatoric strain (confining pressure 0.3MPa)

Figure 4.5.10 presents the motion of particles in unit cells located at macroscopic material points, A and B, which are shown in Fig. 4.5.10(a). Here, Point A corresponds to the material point that undergoes large deformation and reveals the concentration of the macroscopic deviator strain, whereas the strain of Point B is comparatively small. As can be seen from the figure, for the cell located at Point A, velocity vectors and rotation rates become large with increasing total loads, though the rate of apparent axial strain of the overall specimen remains constant. On the other hand, for Point B, there is little motion even after the peak of the apparent stress (the apparent axial strain 2.4%).

Figure 4.5.11 shows the distribution of the normal contact forces between particles, which represents the micro-structural characteristics, associated with macroscopic material points, A and B. Also, in this figure, a line connecting one particle to another gives the contact force between these mutually connected particles and its thickness represents the magnitude of the force. As can be seen from the figure, the normal contact forces exhibit almost isotropic distribution at the initial state and have the same magnitudes for all material points. This is probably due to the nearly isotropic state of macroscopic stress. In the cell located at Point A, the anisotropic distribution of contact forces gradually evolves with increasing load and becomes the most prominent when the apparent axial strain reaches 2.4% in this particular computation. This induced anisotropic nature of the microscopic response is represented by the relatively thicker lines forming the vertical lines and by the thin ones corresponding to the small forces in the horizontal direction. The vertical direction of the transmission of contact forces coincides with that of the maximum principal axis of the macroscopic apparent stress. As for Point B, the anisotropic distribution, which is similar to that in Point A, was observed. However, the distribution of contact forces seems to remain unchanged throughout the deformation process. Thus, the micro-structural characteristics of the cells located at Points A and B differ significantly when the axial strain is 2.4%, though they are similar to each other when the axial strain is small, say 1.0%.

macroscopic material points of the overall structure. Although this feature would be helpful to understand the micro-macro coupling phenomena, we decide to
leave detailed and qualitative investigation of micro-macro coupling behavior to other opportunities because the main purpose of this paper is to propose the two-scale or global-local analysis method for granular media.

4.5.5 CONCLUSIONS

Tremendous amounts of research have been made on the modeling of the macroscopic or phenomenological constitutive laws for granular media. Some of them are incorporated with the micro-scale mechanism of particle motion with reference to micromechanics. However, such prior attempts have been inconclusive. In this context, the multiple scale modeling has been receiving increasing attention in both theoretical and computational mechanics. The two-scale modeling employed in this paper is based on the mathematical homogenization theory for quasi-static equilibrium problems for granular media.

In the proposed global-local analysis method, we prepare the geometrical and physical information about the microstructures that can reproduce the macro-scale material response after averaging the micro-scale structural responses. Therefore, it is not necessary to have a priori the knowledge of the macroscopic or phenomenological material behavior that is usually given as a constitutive law. Such a way of thinking is applicable to various kinds of heterogeneous media. One of the typical applications is the present development for granular media. In the area of computational mechanics, this study must have been the first trial to incorporate the microscopic particulate nature into the global-local computations. Nonetheless, there are some difficulties in modeling the higher order nonlinearities such as non-local effects of deformation. For example, the proposed method cannot simulate the formation of macro-scale slip lines or so-called shear bands caused by macroscopic strain localization. The theoretical and algorithmic developments for simulating such peculiar mechanical behavior should be one of our future studies.

REFERENCE