Discrete element modeling for two-dimensional irregularly-shaped particles and effects of particles shape on mechanical behavior

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ABSTRACT
In order to obtain a precise modeling method that would be comparable to experimental results, the specification of grains such as form, size, elasticity, plasticity should be modeled carefully. Since the shape of the grain affects tremendously the mechanical behavior of total grains like shear resistance, the appropriate modeling of the grain shape is considered to be very important. The method that is employed in this paper is in fact a direct modeling of grain's shape. In this method, the real shape of grain is modeled by combining arbitrary number of overlapping circular elements which are connected to each other in a rigid way. Then a program that is based on discrete element method is used, by making necessary changes to accommodate real grain shape rather than the traditional circular modeling. In order to measure the effects of grains shape on mechanical properties of granular soils, three types of grains, high angular grains, medium angular grains and round grains are considered where several biaxial tests are performed on assemblies with each of grain types. The results emphasize that the angularity of grains is considerably affecting the behavior of soil.

RÈSUMÈ
Pour obtenir une modélisation précise comparable avec des résultats expérimentaux, il faut bien modéliser les caractéristiques de grains tels que la forme, la taille, l'élasticité et la plasticité. Puisque la forme de grains a une influence importante sur le comportement mécanique de l'ensemble de grains comme la résistance au cisaillement, la modélisation appropriée de la figure de grains est très importante. La méthode utilisée dans cette étude est la modélisation directe da la forme de grains. Pour cela, la forme réelle de grains est modélisée en considérant un nombre arbitraire d'éléments circulaires, qui peuvent avoir recouvrement, avec la liaison rigide. Ensuite, un code de calcul en éléments discrets est utilisé en changeant les paramètres essentiels pour que la forme réelle de grains soit engendrée à la place de la forme traditionnelle, autrement dit, circulaire. Pour mesurer l'influence de la forme de grains sur les caractéristiques mécaniques des sols granulaires, trois types de grains ; grains avec une angularité haute, moyenne et grains ronds, sont envisagés et plusieurs essais biaxiaux se font sur un groupe de chaque type de grains. Les résultats montrent que l'angularité des grains a une influence trop importante sur le comportement de sol.

1 INTRODUCTION

In the discrete element method (DEM) scheme proposed by Cundall & Strack (1978), the grains were modeled as discs in 2-D simulations. Simulations with discs have simple calculations; Contact detection doesn't need complicated algorithms. Also in simulations circular grains move easily besides each other, because of easy rotation. But this model has problems in conformity with reality; Resistance to rotation is much less for circular grains compared to that of the actual grains. The internal friction angle of shearing resistance for circular grains modeled using DEM is much less than that of the actual grains with irregular shapes. Also, circular grains have an inherent tendency to roll. On the other hand, the direction of the contact normal forces is always toward the center. So, these forces never contribute to the moments acting on the grains and rotation is only affected of contact tangential forces. Because of these problems, different shapes for grains were proposed to be used in DEM simulations in order to improve simulations.

Many research studies have conducted on the granular soil behavior with elliptical grain's shape so far (Rothenburg & Bathurst 1992, Ting et al. 1993, Ng 1994). Modeling with elliptical grains has these advantages: elliptical grains have fewer tendencies to rotate and simulated mechanical behavior is similar to that of real soils. Ellipse-shaped grain also has a unique outward normal; Generalization of this method to 3-D is simple. Elliptical grains, however, don't accurately represent grain's shapes (Figure 1(a)).

Many researchers have studied the soil behavior with polygon-shaped grains (Barbosa & Ghaboussi 1992, Mirghasemi et al. 1997 & 2002, Matuttis 2000). The results show that a more realistic representation of soil behavior can be achieved. However, this method requires intensive calculation time because of its employed contact detection scheme (Figure 1(b)).

Jensen et al. (1999) proposed the clustering method; In this method, the grain's shape is represented by combining non-overlapping circular elements in a semi-rigid configuration, which is a better representation of grain's shape. The contacts between circular elements are linear-elastic with a high stiffness. Although this method has some improvement over earlier methods, it has problems. The outlines of simulated grain don't resemble those of actual grain. Also, a substantial increase occurs in computational time (Figure 1(c)).

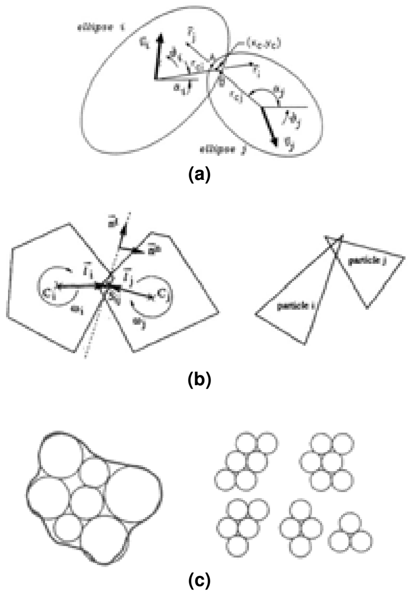

Figure 1. (a) Ellipse-shaped grains, (b) polygon-shaped grains, (c) circular elements combination for modeling grain's shapes in clustering method

In above-mentioned methods, direct modeling of grain's shape is not considered. Because of the considerable effects of grain's shape on mechanical behavior of soils, it seems worthy conducting discrete element method with grains whose shapes are directly modeled.

2 DIRECT MODELING OF GRAIN'S SHAPE

In this method, the real shape of grain is modeled by combining arbitrary number of overlapping circular elements which are connected to each other in a rigid way (Matsushima & Saomoto 2002). Figure 2 shows an example of this method.

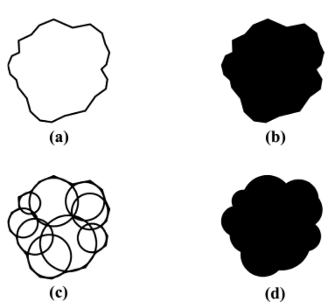

Figure 2. (a) Outline of actual particle, (b) Actual particle (c) Modeling with circular elements, (d) Modeled grain

Figure 2(a) shows outlines of arbitrary grain that is showed in Figure 2(b). Then this method is implemented and circular elements are combined together to model arbitrary grain according to Figure 2(c). It can be seen that created shape with these circular elements shown in Figure 2(d), is very similar to real shape of grain shown in Figure 2(b).

The number of circular elements for modeling grain's shape depends on the degree of non-uniformity and angularity of actual grain's shape, the desired level of accuracy for grain's shape and limitation that is considered for computation time.

This direct modeling method can be used to gain more realistic results for mechanical behavior of granular soils. The results of simulated assemblies of grains can be compared quantitatively with experimental results of actual assemblies. The calculations for simulated assemblies are similar to assemblies with circular grains and complicated algorithm is not required. Generalization of this method to three-dimensional case is simple. The main defect of this method is increase in computation time.

The program "disc" (Bathurst 1985), which is a modified version of "ball" (Cundall 1978), was adopted and modified to simulate assembly of particles which are represented according to above assumption. The program "disc", is used to simulate assemblies of two-dimensional circular-shaped grains and is written on the basis of discrete element method. In this program two major laws are applied: contact law or force-displacement law computes contact forces between circular grains in contact with each other (Figure 3(a)) and application of Newton's second law leads to computation of displacement for each grain. In the changed program, the contact considerations and calculations of contact forces are conducted for each circular element of grain that is in contact with circular element of other grain (Figure 3(b)) and the equation of motion is solved for each grain; with this procedure, rigid connections between circular elements of each grain are obtained without definition of stiffness between these elements.

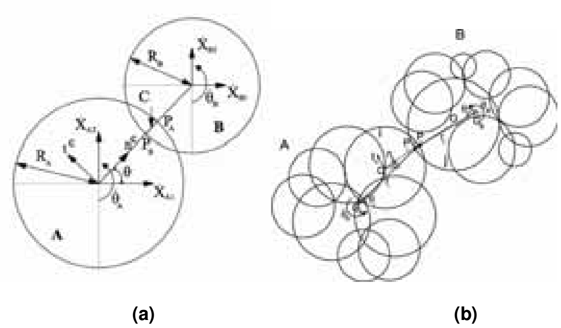

Figure 3. (a) Two circular grains in contact with each other, (b) Two circular elements of two grains in contact with each other

3 THE SELECTION PROCESS OF PARTICLES SHAPE

The above illustrated method is an appropriate tool to investigate the effects of different shapes of grains on mechanical behavior. Three series of grains with different angularity were considered: high angular grains, medium angular grains and round grains. In the first step, 16 types of high angular grains were chosen with equivalent radius ranged from 5mm to 20mm.Then, medium angular grains and round grains were generated through reduction of angularity in high angular grains. In other words, general shape and size of each grain's type was similar for three series as shown in Figure 4.

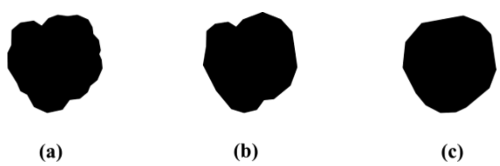

Figure 4. (a) High angular grain, (b) Medium angular grain, (c) Round grain

The results of researches show that grains elongation has considerable effects on mechanical behavior. Elongation is defined as the ratio of the length of a particle to its width. In order to consider only the effects of angularity on behavior, it was tried to minimize the effects of elongation by selecting the grains with equal length and width (elongation equal to 1). In the next step, the grains were modeled by combining circular elements as it was described in part 2.

4 MODELS PREPARATION

In this study, circular assemblies consisting of 1000 grains were used for each series of grains. The grain size distribution of the modeled grains is shown in Figure 5. In this figure, equivalent diameter is the diameter of the equivalent circle having the same area as the grain.

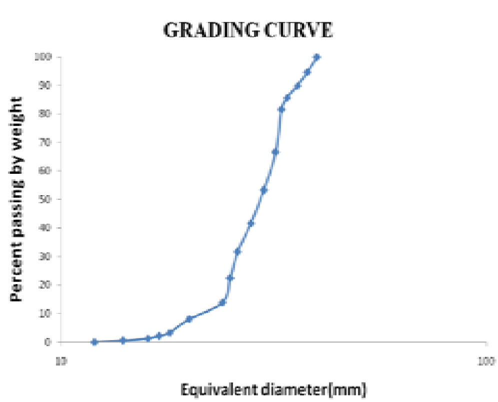

Figure 5. Grain size distribution

At first, circular assembly was generated with high angular grains. Then, the location of gravity center of each grain in the assembly was determined and registered in an output file. For generating assemblies with medium angular grains and round grains, this output file was used and the location of each grain was selected coincident with the location of similar high angular grain. This procedure provides the better comparison between results of assemblies generated with each series of grains. Figure 6 shows the generated assemblies with three series of grains.

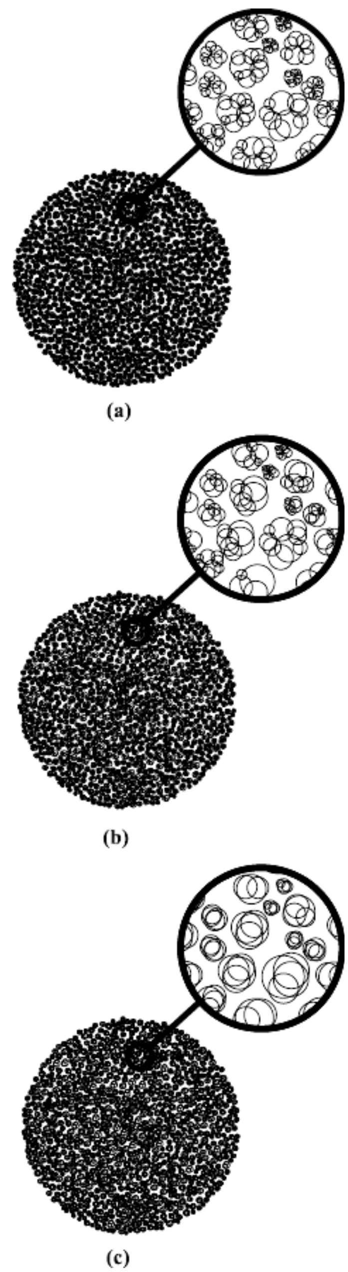

Figure 6. Assemblies generated with (a) high angular grains, (b) medium angular grains, (c) round grains

5 SIMULATED TESTS

In order to consider the effects of different factors on mechanical behavior, two series of tests were conducted on assemblies with each series of grains:
- Tests with different confining pressures
- Tests with different friction coefficients

In this section details of each series of tests are described.

5.1 Tests with Different Confining Pressures

Discrete element method (DEM) parameters used in these tests are listed in Table 1. Normal stiffness and tangential stiffness are used in force-displacement equations for computation of contact forces. Friction coefficient indicates the roughness of grain surface and damping coefficients are defined to dissipate kinetic energy so that static equilibrium condition for assembly of grains can be reached. For better comparison of results, equal parameters were considered for three assemblies.

Table 1.DEM parameters used in simulated tests

Parameters	Values
Normal contact stiffness (N/m)	245×10^7
Tangential contact stiffness (N/m)	245×10^7
Inter-particle friction coefficient	0.5
Inter-particle cohesion	0.0
Density of particles (kg/m^3)	2000
Damping coefficients	5 & 0.01

The simulated tests were conducted in four stages: In the first stage, the generated assemblies were subjected to a strain rate equal to 0.005 in 500,000 cycles to compact initial loose assemblies. In the next stage, zero strain rate was applied in order to bring the assemblies to equilibrium. In stage 3, assemblies were subjected to various isotropic confining pressures (0.1, 0.5, 1, 2 and 4 MPa). In the last stage, biaxial tests were carried out on the assemblies. In the simulated biaxial test, the horizontal stress is held constant and the vertical stress is increased by applying deviatoric strain rate. In this study, the deviatoric strain rate was chosen 0.0005 in the most tests. Only in the cases that assemblies had been subjected to the confining pressure equal to 0.1 MPa, this strain rate led to instability and the strain rate equal to 0.0001 was chosen.

5.2 Tests with Different Friction Coefficients

DEM parameters and their values used in these simulated tests are similar to Table 1 except for the friction coefficient that was chosen variant. The first and two stages of these tests were similar to section 5.1. In stage 3, assemblies were subjected to isotropic confining pressure equal to 1 MPa in various friction coefficients (0, 0.25, 0.5 and 0.75). Also, in the last stage biaxial tests were simulated with different friction coefficients and deviatoric strain rate equal to 0.0005.

6 TESTS RESULTS

The results of simulated tests in this paper are presented in two forms of charts:
- Sin of the mobilized friction angle ($\sin\phi_{mobilized}$) versus axial strain (ε_a)
- Volumetric strain (ε_v) versus axial strain

6.1 Tests Results with Different Confining Pressures

The results of biaxial tests for assemblies with high angular grains in different confining pressures are shown in Figures 7 and 8. Figures 9 and 10 show the comparisons between results of biaxial tests for three series of assemblies in confining pressure equal to 1 MPa. The results for other cases are summarized in Tables 2 and 3.

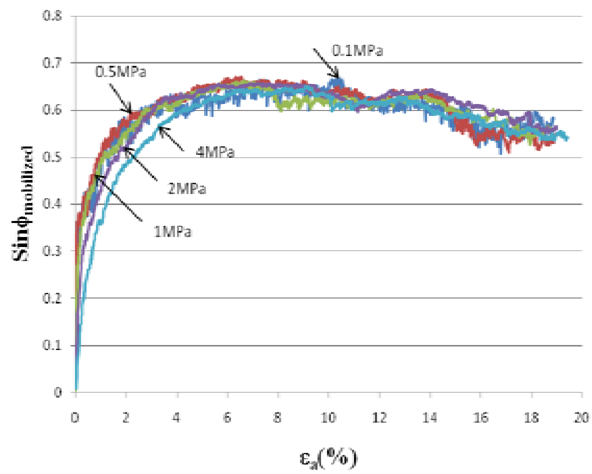

Figure 7. $\sin\phi_{mobilized}$ versus ε_a for assemblies with high angular grains in different confining pressures

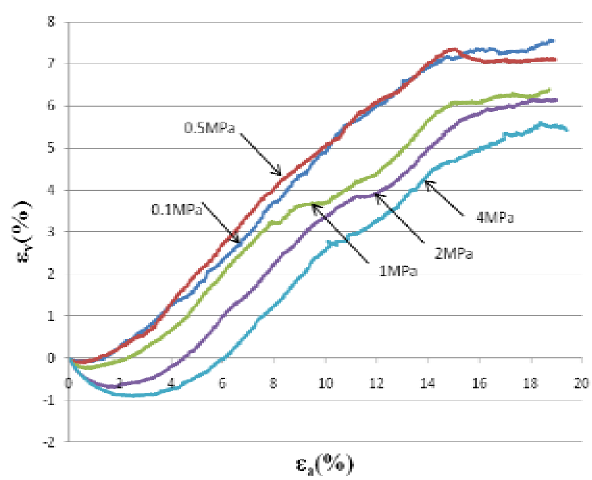

Figure 8. ε_v versus ε_a for assemblies with high angular grains in different confining pressures

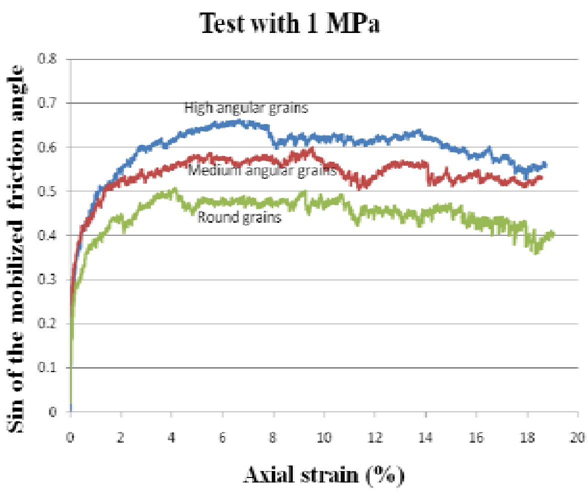

Figure 9. Sin$\phi_{mobilized}$ versus ε_a for three series of assemblies in confining pressure=1MPa

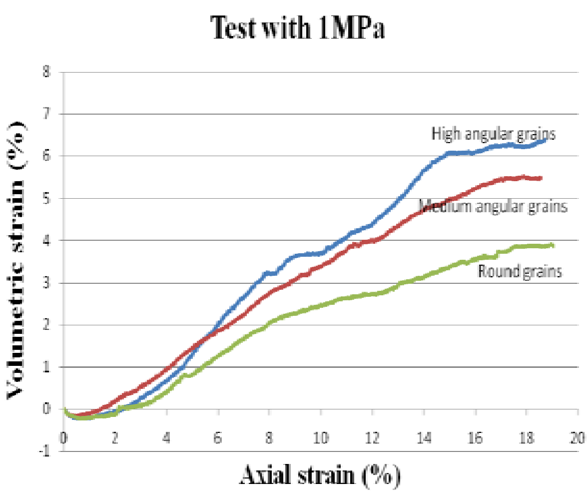

Figure 10. ε_v versus ε_a for three series of assemblies in confining pressure=1MPa

Table 2. $(\phi_{mobilized})_{max}$ values for three series of assemblies in different confining pressures

Confining pressure (MPa)	$(\Phi_{mobilized})_{max}$		
	High angular grains	Medium angular grains	Round grains
0.1	41.8°	39.7°	30.3°
0.5	42.1°	38°	30.8°
1	41.5°	36.8°	30.4°
2	41°	35.8°	28.4°
4	40.5°	36.4°	27.1°

Table 3. Dilation values in ε_a=18% for three series of assemblies in different confining pressures

Confining pressure (MPa)	Dilation value in ε_a=18%		
	High angular grains	Medium angular grains	Round grains
0.1	7.4%	6.6%	3.4%
0.5	7.1%	6.8%	4.1%
1	6.2%	5.5%	3.9%
2	6.1%	5.1%	2.5%
4	5.4%	3.6%	2.4%

The following results were extracted from these charts and tables:

- The shear strength (sin$\phi_{mobilized}$) and dilation decrease with increase in confining pressure. A reduction in both shear strength and dilation at higher confining pressures is attributed to particles breakage (Fumagalli et al. 1970). However, in this study the particles breakage is not modeled; This behavior can be described that the higher confining pressures on the assembly causes to compress it more and does not let it to dilate. So, it doesn't allow particles to move against each other and reduction in shear strength occurs. In general, the more the assembly dilates, the larger the shear strength is. The same results have been obtained in experimental test results.
- In a specified confining pressure, shear strength and dilation increase significantly with increase in angularity. It can be seen that maximum shear strength for high angular and medium angular grains occurred at higher axial strain compared to round grains. As shown, the residual shear strength also increased for assemblies with high angular and medium angular grains compared to assemblies with circular grains. High angular and medium angular grains showed approximately the same residual shear strength in a way that can be implied that the effect of angularity on residual shear resistance decreases at higher angularity.

Shear resistance is due to friction and interlocking between grains. Friction coefficients are assumed the same for three series of assemblies; So, higher shear resistance is due to the higher interlocking between grains. In high angular grains significant interlocking between grains exists and leads to higher shear resistance and dilation of the assembly during performing of biaxial test.

- Numerical results of simulated tests are summarized in Tables 2 and 3. Table 2 shows the maximum of the mobilized friction angle for three series of assemblies in different confining pressures. According to this table, maximum of the mobilized friction angle for high angular grains in a specified confining pressure is approximately 3° to 5° greater than it for equivalent medium angular grains and 11° to 14° greater than it for equivalent round grains. Table 3 shows the values of dilation for three series of assemblies in different confining pressures in axial strain equal to 18%. According to the results, the value of dilation for high angular grains in a specified confining pressure is approximately 0.5% to 2%

and 2% to 4% greater than its value for equivalent medium angular grains and round grains, respectively.

6.2 Tests Results with Different Friction Coefficients

The results of biaxial tests for assemblies with high angular grains in different friction coefficients are shown in Figures 11 and 12. Also, the comparisons between results of biaxial tests for three series of assemblies with friction coefficient equal to 0.75 are shown in Figures 13 and 14. The results for other cases are summarized in Tables 4 and 5.

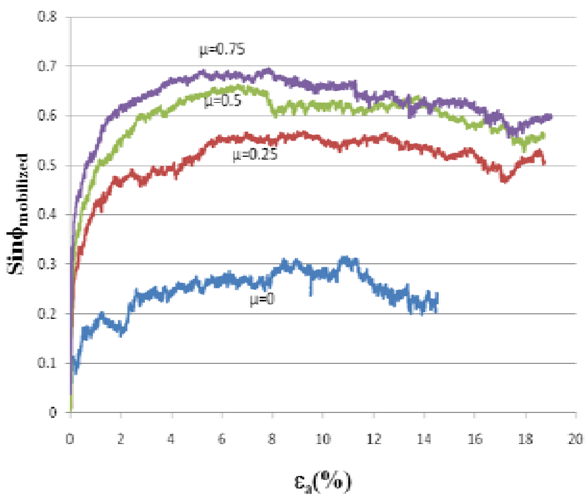

Figure 11. Sin$\phi_{mobilized}$ versus ε_a for assemblies with high angular grains in different friction coefficients

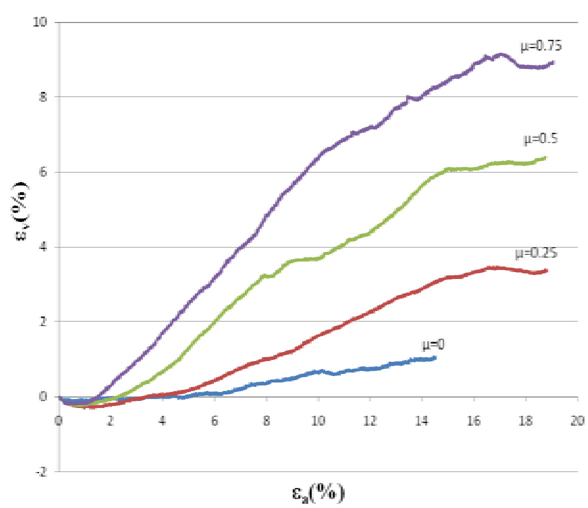

Figure 12. ε_v versus ε_a for assemblies with high angular grains in different friction coefficients

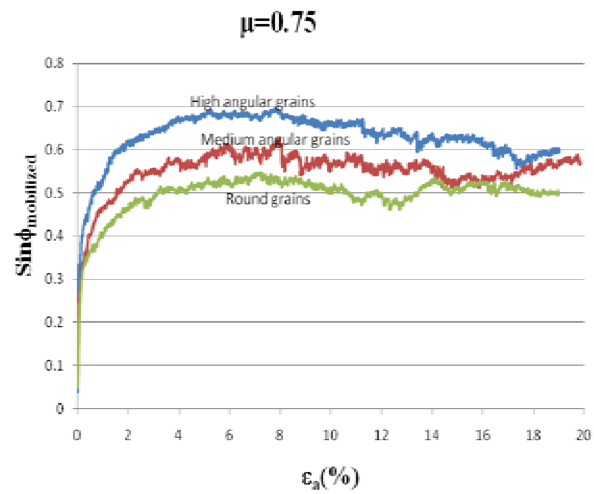

Figure 13. Sin$\phi_{mobilized}$ versus ε_a for three series of assemblies in friction coefficient equal to 0.75

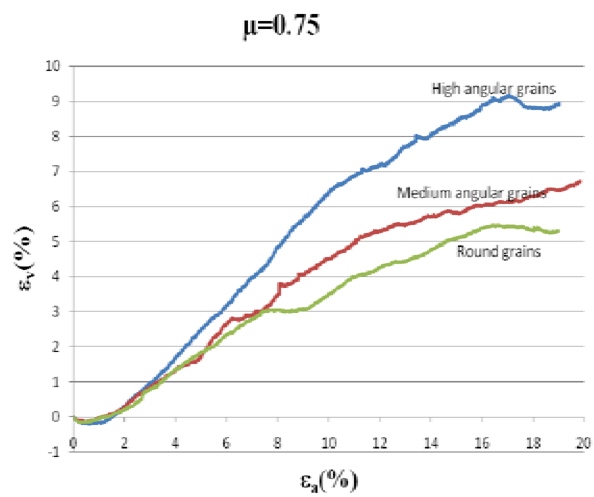

Figure 14. ε_v versus ε_a for three series of assemblies in friction coefficient equal to 0.75

Table 4. $(\phi_{mobilized})_{max}$ values for three series of assemblies in different friction coefficients

Friction coefficient (μ)	$(\Phi_{mobilized})_{max}$		
	High angular grains	Medium angular grains	Round grains
0	18.3°	14.3°	12.9°
0.25	34.6°	30.2°	25.2°
0.5	41.5°	36.8°	30.4°
0.75	44°	38.7°	33.2°

Table 5. Dilation values in ε_a=18% for three series of assemblies in different friction coefficients

Friction coefficient (μ)	Dilation value in ε_a=18%		
	High angular grains	Medium angular grains	Round grains
0	1%	0.5%	0.6%
0.25	3.3%	2%	0.7%
0.5	6.2%	5.5%	3.9%
0.75	8.8%	6.3%	5.3%

The following results were extracts from these figures and tables:

- Shear strength and dilation increase with increase in friction coefficient. It can be seen that the difference between maximum shear strength for friction coefficients equal to 0.5 and 0.75 is small and it can be deduced that the effect of friction coefficient on maximum shear strength decreases at higher values of this coefficient. As shown, with variation of friction coefficient from zero to 0.25, shear strength increases significantly; It demonstrates that frictional strength constitutes considerable portion of shear strength. High angular and medium angular grains show higher increase in shear strength compared to round grains with variation of friction coefficient from zero to 0.25. Also, the residual shear strength increases with increase in friction coefficient. Assemblies with higher friction coefficient show lower decrease in volume and higher dilation during biaxial test. For the case that friction coefficient is equal to zero, dilation is negligible.
- In a specified friction coefficient, shear strength and dilation increase with increase in angularity. Also, the residual shear strength increases with increase in angularity. These results are compatible with results in previous section. In a case that friction coefficient is equal to zero, strength is due to interlocking between grains. In assemblies with high angular grains, higher interlocking between grains leads to higher shear strength compared to assemblies with other series of grains. In medium angular grains, the value of this strength is slightly greater than its value for round grains. Also it can be seen that increase in shear strength with increase in angularity in friction coefficients greater than zero, is more considerable than its increase in friction coefficient equal to zero.
- Numerical results are summarized in Tables 4 and 5. In Table 4, maximum of the mobilized friction angle for three series of assemblies in different friction coefficients is shown. With increasing friction coefficient from 0 to 0.75, maximum of the mobilized friction angle increases 25° for high angular and medium angular grains and 20° for round grains. Also in a specified friction coefficient greater than zero, maximum of the mobilized friction coefficient for high angular grains is approximately 4° to 5° greater than it for medium angular grains and 9° to 11° greater than it for round grains. Table 5 shows the value of dilation for three series of assemblies in different friction coefficients in axial strain equal to 18%. In a case that friction coefficient was zero, assemblies reached to constant volume in lower axial strains; So the values of dilation in this case are due to these lower axial strains. With increasing friction coefficient from zero to 0.75, the value of dilation for assemblies increases approximately 5% to 8%. Also in a specified friction coefficient the value of dilation for high angular grains increases 0.5% to 2.5% and 0.5% to 3.5% compared to its value for medium angular grains and round grains, respectively.

7 CONCLUSION

A method for direct modeling of grains shape was used in this paper. Then three series of grains with different angularities were chosen and modeled with this method. For each series of grains, assemblies consisting of 1000 particles were generated and biaxial tests were conducted on assemblies in different confining pressures and friction coefficients. The results can be summarized as follows:

- For grains with different angularities, mobilized friction angle and dilation decrease with increase in confining pressure.
- In a specified confining pressure shear strength (or mobilized friction angle), dilation and residual shear strength increase considerably with increase in angularities of grains.
- For grains with different angularities shear strength, dilation and residual shear strength increase with increase in friction coefficient.

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