Particuology 9 (2011) 387–397

Contents lists available at ScienceDirect

Particuology

journal homepage: www.elsevier.com/locate/partic

Particle shape consideration in numerical simulation of assemblies of irregularly shaped particles

Saba Abedi, Ali Asghar Mirghasemi *

School of Civil Engineering, College of Engineering, University of Tehran, Tehran P.O. Box 11155-4563, Iran

ARTICLE INFO

Article history:
Received 30 June 2010
Received in revised form
23 November 2010
Accepted 30 November 2010

Keywords:
Discrete element method
Granular soil
Angularity
Confining pressure

ABSTRACT

The mechanical behavior of granular materials depends much on the shape of the constituent particles. Therefore appropriate modeling of particle, or grain, shape is quite important. This study employed the method of direct modeling of grain shape (Matsushima & Saomto, 2002), in which, the real shape of a grain is modeled by combining arbitrary number of overlapping circular elements which are connected to each other in a rigid way. Then, accordingly, a discrete-element program is used to simulate the assembly of grains. In order to measure the effects of grain shape on mechanical properties of assembly of grains, three types of grains—high angular grains, medium angular grains and round grains are considered where several biaxial tests are conducted on assemblies with different grain types. The results show that the angularity of grains greatly affects the behavior of granular soil.

1. Introduction

Published data show that particle shape has considerable influence on the engineering properties of granular soils. Tests conducted by Holubec and D'Appolonia (1973) on medium to fine sands with varying particle shapes indicated that granular materials with the same relative density could have different mechanical behavior due to angularity. They concluded that the variation of engineering properties due to particle shape could be of the same order of magnitude as the variation of properties due to changes in relative density, thus suggesting that particle shape could be considered an index property to correlate the properties of granular materials.

Rothenburg and Bathurst (1992) reported the results of numerical simulations of planar assemblies of elliptical particles. Packing simulations of the initial assembly showed that, for ellipses with eccentricities up to about 0.2, the coordination numbers of the generated assemblies increased with increasing eccentricity. The resultant peak angle of internal friction in biaxial shear simulations showed the same trend and correlated well with the initial coordination number. Ting, Khawaja, Meachum, and Rowell (1993) reported similar conclusion from isotropic compression and biaxial shear test simulations on assemblies of two-dimensional elliptical particles.

By means of numerical simulations of assemblies of polygon-shaped particles, Mirghasemi, Rothenburg, and Matyas (2002) concluded that particle angularity had an important effect on the compressibility and shear strength of the granular media.

In order to obtain a precise modeling method that would be comparable with experimental results, the specifications of grains such as form, size, elasticity, plasticity should be modeled carefully. Since the shape of the grain affects tremendously the mechanical behavior of granular media such as shear resistance, appropriate modeling of grain shape is considered very important.

In the early discrete element method (DEM) scheme presented by Cundall and Strack (1979), the grains were modeled as discs in 2D and as spheres in 3D simulations with the advantage of simplicity in calculation: contacts between grains can be detected with simple algorithms, and in the simulated tests circular or spherical grains can move and rotate easily, though not without problems in conforming reality. The internal friction angle of shearing resistance is much less for circular or spherical grains compared to that of actual grains with irregular shapes. Resistance to rotation for circular or spherical grains is much less than that of actual grains, particularly for grains with inherent tendency to roll. On the other hand, the direction of the normal contact forces is always toward the center; these forces, however, never contribute to the moments acting on the grains, rotation being only affected by tangential contact forces. Because of these problems different shapes for grains were presented for use in DEM simulations in order to improve the results of simulation. In most cases of modeling that have been applied so far, grain form is generally considered elliptical,

* Corresponding author. Tel.: +98 21 66957783; fax: +98 21 66957787.
E-mail address: aghasemi@ut.ac.ir (A.A. Mirghasemi).

1674-2001/$ – see front matter
doi:10.1016/j.partic.2010.11.005

Nomenclature

A	total area of the assembly
A_s	area occupied by grains in the assembly
A_V	void area between grains in the assembly
F_i	grain unbalanced force
f_i^C	contact force vector
F_n	normal contact force between two particles
ΔF_n	Incremental normal contact force
F_s	shear contact force between two particles
ΔF_s	incremental shear contact force
I	grain moment of inertia
K_n	grain stiffness in normal direction
K_s	grain stiffness in shear direction
l_j^C	contact length vector
m	grain mass
M	grain resultant moment
Δn	relative normal displacement at a contact
Δs	relative shear displacement at a contact
SF	shape factor
$\ddot{x}_i$	grain translational acceleration
$\ddot{\theta}$	grain rotational acceleration
$\phi_{mobilized}$	mobilized friction angle
σ_1, σ_2	major principal stresses
σ_{ij}	stress tensor
ε_a	axial strain
ε_v	volumetric strain

ellipsoidal, polygonal, etc., none of which, however, directly models any irregularly shaped grain, hence will not project the expected mechanical behavior, thus pointing to the need of direct modeling of grains with irregular shapes.

2. Methods for modeling grain shape

2.1. Brief review of particle shape modeling

Many researchers studied granular soil behavior in terms of ellipse-shaped grains in 2D and ellipsoid-shaped grains in 3D simulations (Bagherzadeh-Khalkhali & Mirghasemi, 2009; Lin & Ng, 1997; Ng, 1994; Rothenburg & Bathurst, 1992; Ting et al., 1993), apparently with the following advantages: grains have unique outward normal so calculations of forces are simple; grains have fewer tendencies to rotate, making simulated mechanical behavior similar to that of real soils. Such modeling, however, does not accurately represent the shape of grains (Fig. 1(a)).

Many studies considered granular soil behavior in terms of polygon-shaped grains (Bagherzadeh-Khalkhali, Mirghasemi, & Mohammadi, 2008; Barbosa & Ghaboussi, 1992; Matuttis, Luding, & Herrmann, 2000; Mirghasemi, Rothenburg, & Matyas, 1997; Mirghasemi et al., 2002; Seyedi Hosseininia & Mirghasemi, 2006, 2007), to show rather realistic representation of soil behavior (Fig. 1(b)), though the method is time-consuming.

Potapov and Campbell (1998) proposed the elliptical approximation with oval-shaped boundaries determined by four continuously jointed circular arches. This method involves simple calculations because contacts between two circular segments of grains are similar to contacts between circles in the original DEM code. The results of simulated tests using this method show that this method is effective; though the real shape of the grain is not effectively represented (Fig. 1(c)).

In the method presented by Favier, Abbaspour-Fard, Kremmer, and Raji (1999) to model axi-symmetrical grains, particles are modeled by combining multiple overlapping spheres with fixed inner-sphere connections. Simulations with this method showed good agreement with experimental results. This method can model any shape of grains, unless they are highly angular (Fig. 1(d)).

Jensen, Bosscher, Plesha, and Edil (1999) presented a clustering method in which the grains are modeled by combining non-overlapping circular elements in a semi rigid configuration; The contacts between circular elements are linear-elastic with a high stiffness. Although this method has some improvement over earlier methods, the outlines of simulated grain do not resemble those of the actual grains. Also computational time is long (Fig. 1(e)).

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

2.2. Direct modeling of grain shape

In this method, the real shape of a grain is modeled by combining an arbitrary number of overlapping circular elements which are connected to each other in a rigid way. Fig. 2 shows a simple algorithm to find the optimized number of circular elements to model the real shape of a grain (Matsushima & Saomto, 2002; Matsushima, Hidetaka, Matsumoto, Toda, & Yamada, 2003), the resulting outline closely coinciding with that of the real grain (Fig. 3).

Fig. 3(a) shows the outline of an arbitrary grain that is shown in Fig. 3(b). By combining overlapping circles, closely real shape of the grain is generated (Fig. 3(c)), showing that the created shape with circular elements (Fig. 3(d)) closely resembles the real shape of the grain shown in Fig. 3(b).

The actual shape of a grain can be precisely modeled with a maximum of 10–15 circular elements. The number of circular elements for modeling a grain shape depends on the degree of non-uniformity and angularity of the actual grain shape, the desired level of accuracy for the grain shape and the limitation of computation time.

This direct modeling method can be used to realize realistic results for mechanical behavior of granular soils. The results of simulated assemblies of grains have been compared quantitatively with experimental results of actual assemblies (Matsushima & Saomto, 2002). The calculations for simulated assemblies are similar to assemblies with circular grains, for which no complicated algorithm is required.

The program DISC (Bathurst, 1985), which is a modified version of BALL (Cundall, 1978) is adopted and modified to simulate assembly of grains with real shape. This program, calls for the Newton's second law to compute displacements for each grain from the current resultant forces and the moments acting on the grain, as follows:

$$\sum F_i = m\ddot{x}_i, \quad i = 1, 2$$
$$\sum M = I\ddot{\theta}, \qquad (1)$$

where F_i is the unbalanced force on each grain, M is the resultant moment on each grain, m is the mass of the grain, I is the moment of inertia of the grain, and $\ddot{x}_i$ and $\ddot{\theta}$ are the grain accelerations. For each grain, accelerations are integrated over small time-steps to give velocities and displacements. The time-step is chosen small enough that the velocities and accelerations can be assumed constant over it. The calculated displacements are used in contact law or force–displacement law through which the con-