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Research Paper

Discrete element modeling of crushable sands considering realistic particle shape effect

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A B S T R A C T

This study proposed a novel approach for generating crushable agglomerates with realistic particle shapes in discrete element modeling (DEM). The morphologies of sand particles were obtained by X-ray micro-computed tomography scanning and image processing. Based on the particle surface reconstructed by spherical harmonic analysis, the crushable agglomerates with realistic particle shapes can be generated in DEM simulations. The results of single particle crushing tests showed that particle shapes significantly influence the fracture patterns and crushing strengths of sand particles. Furthermore, two one-dimensional compression tests were conducted to investigate the particle shape effect on micro- and macro-mechanical behaviors of crushable sands.

1. Introduction

Particle shape and particle crushing are inherent soil characteristics that determine the mechanical properties of granular soils. It is generally acknowledged that particle shape dominates the mechanical behaviors of sands under low stress conditions, while particle crushing dominates the mechanical behaviors of sands under high stress conditions. A large amount of experimental studies has shown that particle shape highly influences the compressibility, shear strength, shear-induced dilatancy, and local shear failures of sands [1–3]. Meanwhile, other high stress experiments have found that particle crushing gives rise to the evolution of a distribution of particle sizes, and this in turn controls the yielding, hardening, softening, and critical state behaviors of sands [4–6]. At the particle scale level, it is easy to understand that the local features of the particle shape will highly increase the stress concentration inside of the particle subjected to its contact forces. This stress concentration is the incentive to crush the particle when its magnitude is larger than the strength of the internal joints and fissures. For this reason, it is critical to understand the fundamental micromechanisms of the particle shape effect on sand crushability under high stress conditions.

In order to elucidate the effect of particle shape on particle crushing behaviors of granular materials, Cavarretta et al. [7] conducted a series of one-dimensional (1D) compression tests on intact and crushed ballotini samples. The results revealed that crushed samples have lower yield stress and higher plasticity than that of intact samples, which means that irregular ballotinis have lower strengths and higher breakage than those of spherical ballotinis. Due to the limitations of experimental techniques, few experimental studies exist that investigate the micromechanisms of the particle shape effect on particle crushing behaviors of natural sands under high stress conditions. As an alternative, the discrete element method (DEM) [8] has made significant contributions towards identifying the fundamental micromechanics of crushable sands over the past two decades.

Aided by DEM, three basic methods have been proposed to simulate the crushing behaviors of sand particles. The first method was proposed by Potapov and Campbell [9], which simulates the crushing process by including internal structure in the form of tetrahedral meshes, and allows the elements to separate. The second method bonds a group of elementary balls together to form a porous agglomerate, which can disintegrate to simulate particle breakage. It has been widely used by a number of geotechnical researchers [10–16] to investigate a wide range of fundamental soil behaviors, including soil yielding, plastic deformation, grading evolution, strain localization, particle-scale energy allocation, etc. The third method, proposed by Lobo-Guerrero and Vallejo [17,18], simulated particle breakage by replacing the original particle by a cluster of arranged smaller fragmental particles. The authors [19] further developed this method by introducing a

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probabilistic fracture criterion of particle breakage, considering the size effect and contact configuration of the particle. However, it should be noted that both of the methods possess an apparent limitation, which is the neglect of the particle shape effect on the particle crushing process.

To take the particle shape effect on particle crushing behaviors in numerical simulations into account, Ueda et al. [20] proposed a cutting method to generate crushable agglomerates with various idealized shapes within a two-dimensional (2D) DEM framework. Within three-dimensional (3D) DEM framework, Cleary and his coworkers [21,22] proposed to generate a very dense packing of progeny inside the bounding parent super-quadric to construct a non-round rock particle, which can be broken into non-round progeny by an energy based fracture criterion. In the context of a combined finite-discrete element method (FDEM), Ma et al. [23,24] proposed a 3D cohesive crack model to simulate the particle breakage of convex-shaped granular materials. Most recently, based on the 3D laser ranging technique, Ma et al. [25] developed the FDEM to investigate the crushing behaviors of individual natural rock particles with concave shapes subjected to uniaxial compressions. Due to the computation cost of FDEM, simulating crushing behaviors of large scale sand samples incorporating the effect of realistic particle shapes still remains a challenge.

In the past two decades, the development of X-ray micro-computed tomography (μCT) technology has provided a powerful tool for the 3D visualization and characterization of the microstructure and micromorphology of natural sand particles [26–28]. The application of μCT technology enables researchers to incorporate realistic particle shapes in DEM simulations. In this context, the first step is to reconstruct the accurate particle surface based on the μCT images. The conventional method has been applying image processing techniques, including detecting boundary voxels, marching cubes, and smoothing surface mesh [27,28]. A more sophisticated method has been widely acknowledged by means of the mathematical spherical harmonic (SH) function to reconstruct the smooth and continuous particle surface [29–32]. Based on the reconstructed particle surface, Ferellec and McDowell [33] proposed an optimized clump logic approach to approximately simulate sand particles with realistic shapes by using DEM. Alternatively, Andrade and his group [34,35] used the granular element method, an advanced DEM combined with non-uniform rational basis-splines, to capture complex particle shapes of natural sands. However, the particles generated by these methods are rigid and uncrushable during the loading process.

The objective of this study was to propose a novel approach for generating crushable sands with realistic particle shapes within a 3D DEM framework, and further to investigate the effect of the realistic particle shape on particle crushing behaviors of natural sands subjected to 1D compression. To achieve this objective, high resolution X-ray scanning was firstly conducted to obtain μCT images of a pile of natural sand particles, i.e., Leighton Buzzard sand (LBS) particles. A series of image processing techniques were then applied to the μCT images to extract the morphologies of all individual particles. The 3D surface mesh of each sand particle was then reconstructed by using the SH analysis proposed in an earlier study by the authors [31,32]. Based on the reconstructed particle surface mesh, a generation framework for crushable agglomerates with realistic particle shapes was mainly established in the DEM platform PFC^{3D} [36]. In order to validate the efficiency of the proposed method and calibrate the physical parameters within DEM simulations, a series of single particle crushing tests were conducted on spherical particles and realistic-shaped particles. Finally, two sand samples containing spherical agglomerates and realistic-shaped agglomerates were generated to investigate the particle shape effect on particle crushing behaviors during 1D compression.

2. Particle surface reconstruction

2.1. μCT scanning and image processing

LBS is quarried near the town of Leighton Buzzard in southeast England. It is from the lower Greensand sequence, which was deposited in shallow sea and estuarine environments. The mineralogy is predominantly quartz with some feldspar, and is characterized by chemical inertness and considerable hardness. The

Fig. 1. Preparations for the μCT scanning of sand particles: (a) selected LBS particles; (b) microtube specimen containing the LBS particles fixed with silicon grease; and (c) rotation unit base for the microtube specimen subjected to X-ray scanning.