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Mechanics of granular and polycrystalline solids

Modeling the influence of particle morphology on the fracture behavior of silica sand using a 3D discrete element method

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ABSTRACT

The constitutive behavior and deformation characteristics of uncemented granular materials are to a large extent derived from the fabric or geometry of the particle structure and the interparticle friction resulting from normal forces acting on particles or groups of particles. Granular materials consist of discrete particles with a fabric (microstructure) that changes under loading. Synchrotron micro-computed tomography (SMT) has emerged as a powerful non-destructive 3D scanning technique to study geomaterials. In this paper, SMT was used to acquire in situ scans of the oedometry test of a column of three silica sand particles. The sand is known as ASTM 20–30 Ottawa sand, and has a grain size between US sieves #20 (0.841 mm) and #30 (0.595 mm). The characteristics and evolution of particle fracture in sand were examined using SMT images, and a 3D discrete element method (DEM) was used to model the fracture behavior of sand particles. It adopts the bonded particle model to generate a crushable agglomerate that consists of a large number of small spherical sub-particles. The agglomerate shape matches the 3D physical shape of the tested sand particles by mapping the particle morphology from the SMT images. The paper investigates and discusses the influence of agglomerate packing (i.e., the number and size distribution of spherical sub-particles that constitute the agglomerate) and agglomerate shape on the fracture behavior of crushable particles.

1. Introduction

Sand particle fracture has been extensively investigated by many researchers due to its profound influence on the behavior of sand. It has been examined at different scales, ranging from single particle level to laboratory specimen size. Researchers mainly adopted experimental, analytical, and numerical approaches to better understand and characterize the underlying micro-mechanics of particle fracture (e.g., [1–3]). Discrete Element Modeling (DEM) is a common discontinuum numerical method allowing one to model the breakage of particles in granular materials. The crushable nature of sand particles is generally represented using two common methods within the framework of DEM. The first method replaces a broken particle with a group of smaller particles based on a pre-defined failure criterion [4]. In the second method, researchers used an agglomerate composed of many bonded spherical sub-particles to represent the sand particles [5–8]. These studies provided a valuable contribution to the literature, allowing a better understanding of the fundamental behavior of crush-

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able particles, but none of the techniques already published could reproduce the 3D particle shape in DEM environment. Recently, Cil and Alshibli [9] proposed to use hexagonal and cubic packings of bonded spherical particles to generate an agglomerate in order to closely match the 3D physical shape of the particle. In this paper, the evolution of particle fracture and specimen deformation is investigated using a 3D DEM model with crushable agglomerates that match the 3D physical shape of silica sand particles via Synchrotron Micro-computed Tomography (SMT) images. This paper focuses on the improvement of the approach proposed by Cil and Alshibli [9] by adopting a different packing scheme, and investigates the characteristics of the particle fracture in granular materials by considering the variations in the distribution of spherical sub-particle sizes and in agglomerate packing.

2. Synchrotron Micro-computed Tomography (SMT) scans

SMT is a non-destructive in situ visualization technique that yields 3D high-resolution images of specimen by mapping X-ray attenuation data. SMT scans were acquired at GeoSoilEnviroCARS (GSECARS) Sector 13 of the Advanced Photon Source (APS), Argonne National Laboratory (ANL), Illinois, USA, a state-of-the-art synchrotron facility that provides a collimated and tunable high-energy X-ray beam. In a typical SMT setup, the specimen is positioned between the incoming X-ray source and detector system. As the X-rays travel through the specimen, some of the photons are absorbed by it, which depends on the chemical composition and the X-ray energy level. A scintillator is used to convert the transmitted X-rays to a visible light that is recorded using a CCD camera system. Each image provides attenuation data for a particular angle. A series of projection images needs to be acquired at different angles by rotating the specimen about an axis perpendicular to incident beam. The raw SMT data are processed to obtain the 3D spatial distribution map of the X-ray attenuation of the specimen, which is composed of stacks of 2D images.

In this study, SMT scans were acquired for a column composed of three sand particles that were subjected to 1D compression using beam-13D of APS. A special test cell that consists of a loading system, a specimen mold, load cells, and a data acquisition system was used in the experiments. The sand is ASTM 20-30 Ottawa sand; a natural silica sand with well-rounded particles that has a grain size between US sieves #20 (0.841 mm) and #30 (0.595 mm). To prepare a specimen, the sand particles were poured into a 1-mm cylindrical hole at the center of a 15-mm acrylic cylindrical mold and were compressed at a constant displacement rate of 0.2 mm/min. The SMT scans were acquired at an energy level of 23 keV that produced images with a spatial resolution of 4.95 μm/pixel. The sand column was scanned before applying the load; it was then loaded until the desired compressive load was reached, and another scan was performed while pausing loading. This procedure was repeated for consecutive load levels and scans. Fig. 1 shows an example load versus displacement relationship and axial cross sections of the 3D SMT images of the specimen at different displacement levels. Fig. 1a shows that the compressive load increases gradually as compression progresses. Some small load drops are observed due to particle movement and/or local asperity damage at particle contacts before the major fracture of one of the particles, which resulted in a significant drop in the load. Multiple small drops in load emerged after the initial fracture, which resulted from the continuous fracture of broken fragments of the fractured particle. The SMT images shown in Fig. 1b clearly illustrate the compressive behavior of sand particles under 1D compression. Initially, particles slightly rearrange through rotation and/or translation, and reach a stable configuration in which lateral support is provided by the mold walls. Then, the column of particles resists the increasing compressive load until fracture occurs in the form of catastrophic splitting. Both fractured and intact particles continue to fracture as the compression progresses.

3. DEM simulations

SMT images are 3D array structures that contain the spatial distribution map of the X-ray attenuation of the specimen. Raw scan data need to be analyzed to extract the 3D sand particle morphology. The first step in image analysis is to identify and separate each constituent material in the image, which was performed with the help of a segmentation process using Avizo Fire commercial software. Using the thresholding approach, SMT image was binarized by assigning a value of 1 for the sand particles and a value of 0 for the rest of the image, including the loading platens and acrylic cylindrical mold. Then, the 3D segmented binary image was saved as a text file to transfer particle shape information to PFC3D DEM software. The 3D view of the sand particles after segmentation is shown in Fig. 2b.

The 3D physical shapes of the silica sand particles were reproduced in DEM environment with the help of 3D SMT images. Initially, a prismoidal container was generated and filled with spherical particles that have a uniform grain size distribution defined by a minimum radius ($R_{\min}$) and a maximum radius ($R_{\max}$). The dimensions of the rectangular container were determined based on the dimensions of the 3D volume file of the SMT image (Fig. 2a). Then, the specimen was subjected to a relatively small isotropic compressive stress condition to obtain a densely packed specimen. After that, prismoidal DEM assembly and 3D segmented SMT image were compared in 3D space, and DEM particles that are corresponding to void space in segmented SMT image were deleted from the assembly (Fig. 2c). DEM particles corresponding to the volume occupied by silica sand particles in segmented SMT image were identified and categorized based on the corresponding sand particle. Then, the coordinates and radii of spherical sub-particles for each agglomerate were saved in a text file which is called an agglomerate template.

Sand particles were represented with agglomerates of bonded particles. Agglomerates were generated in a 1D compression test simulation using the position and size information of the spherical sub-particles in the agglomerate template files.