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Research paper

Determination of microscopic parameters of quartz sand through tri-axial test using the discrete element method

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ABSTRACT

A calibration procedure, in which coupled effects of microscopic parameters are considered, is proposed to determine the values of the microscopic parameters in the Discrete Element Method (DEM) for Fujian quartz sand. Laboratory tri-axial tests are conducted to be compared with the DEM simulations and the effects of end restraint in the laboratory tests are eliminated through a digital image measurement system. Sensitivities of the macroscopic behaviour of the specimen to the microscopic parameters are analyzed through DEM simulations. Four coupled effects of the microscopic parameters on the macroscopic behaviour are investigated through a graphic method and then considered in the calibration procedure.

1. Introduction

Granular sands cover a broad area of research on geotechnical engineering including foundation engineering, slope stability, and earthquake liquefaction, etc. The local discontinuous nature plays an important role in the mechanical behaviour of granular matter [14]. As a kind of granular material, sand shows complex features in geotechnical engineering such as anisotropy [2], dependency of stress history [7], and Reynolds dilation [31,30]. These features are difficult to be understood from points of continuum mechanics. The discrete element method (DEM) [9], in which each grain is modelled individually, can describe the discontinuous behaviour of sands easily. So it has been increasingly popular in geotechnical engineering in recent years [17,38,10,28]. In DEM simulations, the microscopic parameters of particles should be specified so that the aggregation of particles can reproduce the behaviour of real granular sands. The accuracy of DEM models depends largely on the choice of micro-parameters [12]. So the determination of microscopic parameters of sand particles is a crucial issue for the applications of DEM in geotechnical engineering.

Some researchers have tried to obtain the microscopic parameters of a single sand particle, such as the Young's modulus and the inter-particle friction coefficient, through laboratory tests. The Young's modulus of sand particles can be obtained by nanoindentation [39]. But these tests only provide a reasonable range of the Young's modulus of particles [39] and can hardly be utilized in the DEM simulations directly. Jones et al. [23] have used the atomic force microscope (AFM) to measure the inter-particle friction coefficient of artificial particles. The size of these artificial particles varied in the range of 0.04–0.20 mm. However, the precision of the AFM, the need of complex calibration, and its cost bring about difficulty in its application for measuring the inter-particle friction of sand particles [16]. Cavarretta et al. [8] have invented an apparatus to measure the inter-particle friction coefficient between sand-sized grains. This device has advantages of simplicity of sample preparation, reliability of calibrations, and moderate cost compared with AFM. However, for tests with fine particles that are regular in shapes, the operation of the apparatus is rather complicated [13]. Moreover, even if the direct measurement of microscopic parameters is possible, the accuracy of DEM simulations with these measured parameters depends on the accurate modelling of particle shape and particle size and on the accurate representation of the contact behaviour in DEM [3]. As it is difficult to model the particle size and particle shape accurately [11] and the contact behaviour is often simplified in DEM due to the computational limitations, such properties as the Young's modulus and sliding friction coefficient of sand particles measured through laboratory tests can only provide a reference and can hardly be implemented in DEM simulations directly. Therefore, many researchers use the trial-and-error method [5,15] to calibrate microscopic parameters in the DEM.

When the trial-and-error method is utilized for calibration, simple laboratory tests (such as the natural angle of repose test [44],

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the direct shear test [33], and the tri-axial compression test [5] are simulated by DEM and microscopic parameters are determined through the relationships between microscopic parameters of particles and macroscopic responses of the specimen. In view of the advantages of the tri-axial compression test such as the widespread use in the geotechnical laboratory, the relative clarity of the stress state (axis-symmetric stress state) and the standard operating procedure, this laboratory test was often utilized for parameter calibrations in DEM [5,41,25]. Therefore, the tri-axial compression test was used for the calibration of microscopic parameters in this study.

In the interest of the calibration, the effects of the microscopic parameters on the macro behaviour of the specimen in the tri-axial test have been studied by several researchers [5,25]. Coupled effects of the microscopic parameters on the macroscopic behaviour have been found by Belheine et al. [5]. This makes the calibration procedure more complex and therefore a simplified calibration method was proposed by Belheine et al. [5]. This method has been widely used by other researchers. However, in Belheine's method, the coupled effects of microscopic parameters, such as the couple effect of the rolling friction and sliding friction on the dilation angle of the specimen, were underestimated during calibration. This makes the calibration procedure clear and simple, but the simplification may also influence the accuracy of the calibration. Therefore, a calibration procedure based on the tri-axial test, in which the coupled effects can be considered, is still in demand.

In the laboratory tri-axial test, the end restraint caused by the frictional top and bottom boundaries would greatly affect the stress state and the volumetric strain of the specimen. If the end restraint is considered in DEM simulations, it will make the calibration procedure complicated and even infeasible. So a better thought is to eliminate the effect of the end restraint in the laboratory tri-axial test. To this end, the lubrication of top and bottom plates using rubber membranes with silicone grease in between [6] is often utilized. However, the end lubrication has its drawbacks that the complex operation of end-lubricated tri-axial test usually makes specimen easily disturbed and the existence of end lubrication makes the specimen tend to slip during shearing. In this study, a digital image measurement system based on the conventional tri-axial apparatus, which is developed by Liu et al. [27] and Shao et al. [34] to overcome the drawbacks of the end-lubricated tri-axial test, was employed to serve the calibration of microscopic parameters. Through the digital image measurement system, the deformation of middle part of the specimen, which is observed to be uniform [27], was recorded. Meanwhile, the shear stress on the cross section of the middle part was demonstrated to be negligible. The behaviour of the middle part of the specimen was taken into account in the calibration. Then the effect of the end restraint can be eliminated by excluding the deformations in the vicinity of the two ends of the specimen in the tri-axial test.

The numerical simulations were performed using Open Source DEM code LIGGGHTS [24]. In our DEM simulations, spheres were utilized to model the sand particles. Hertz-Mindlin model [33] was used to describe the contact behaviour of particles. To represent the interlocking due to irregular particle shape [40], the rolling contact model was employed. Particle diameters were scaled up to reduce the number of particles and thereby ease the computational burden. A series of numerical tests were performed to evaluate the effect of micro-parameters on the macroscopic behaviour of the sand specimens. A graphic approach was proposed to investigate the coupled effects of microscopic parameters on the macroscopic behaviour of the specimens. The aim of this study is to propose a method, in which the coupled effects of microscopic parameters are considered, to calibrate the micro-parameters of Fujian quartz sand used in DEM through the tri-axial test. And it further examines the capability of the discrete element method to model the macroscopic behaviour of sand.

2. Laboratory tri-axial tests

2.1. The digital image measurement system

The digital image measurement system is developed based on a conventional tri-axial test apparatus. As shown in Fig. 1, it is composed of Pressure Cell, Complementary Metal-Oxide-Semiconductor (CMOS) Camera, Camera Bracket, and Scalable Camera Bellows. The CMOS camera, coupled with two reflection mirrors, is used to obtain images of the entire surface of the specimen at the recording instants. The membrane surrounding the specimen is printed with white and black grids of 7×7 mm^2, as shown in Fig. 2 (front view of the membrane is displayed herein). The nodes of the white and black grids are identified via a sub-pixel corner detection algorithm [36] as shown in Fig. 2. The displacements of these nodes are evaluated through comparisons of pictures of the specimen recorded at certain instants. Then the strains of the entire surface of the specimen can be determined by taking each grid as a four-node iso-parametric element [34]. The details of the digital image measurement system are described in Refs. [27,34].

2.2. Characterization of the middle part

In the digital image measurement system, to obtain the stress-strain and volumetric strain-strain responses of the middle part of the specimen, the specimen is divided into several layers as shown in Fig. 3. A computational region, in which the data will be processed, is predefined. In the following calculation, one row of white grids (with black grids in between) or one row of black grids was considered as one layer. As such, there are eleven layers in the computational region. The height of the computational region is 77 mm. It is 3 mm shorter than the whole specimen of 80 mm in height and 39.1 mm in diameter. The axial and radial strains of each grid can be calculated according to the displacement of the grid nodes. Then the representative axial and radial strains of every layer can be calculated through averaging of the corresponding axial and radial strains of grids in this layer. The details of the calculation are described in Ref. [27,34].

The representative axial and radial strain of the ith layer is written as ε_{ai} and ε_{vi}, respectively. Assuming that every layer maintains a cylindrical shape during deformation (this is reasonable when every layer is thin enough for consolidated drained tri-axial test), we can calculate the representative volumetric strain of the ith layer as following:

$$\varepsilon_{vi} = (1 + \varepsilon_{ai})(1 + \varepsilon_{ri})^2 - 1 \tag{1}$$

In the present study, we will consider the response of the middle three layers (21 mm in height) of the specimen as illustrated in Fig. 3. The representative axial, radial, and volumetric strains of the middle three layers are determined as following:

$$\varepsilon_{3a} = \frac{\varepsilon_{a5} + \varepsilon_{a6} + \varepsilon_{a7}}{3} \tag{2}$$

$$\varepsilon_{3r} = \frac{\varepsilon_{r5} + \varepsilon_{r6} + \varepsilon_{r7}}{3} \tag{3}$$

$$\varepsilon_{3v} = \frac{\varepsilon_{v5} + \varepsilon_{v6} + \varepsilon_{v7}}{3} \tag{4}$$

where ε_{3a}, ε_{3r}, and ε_{3v} are the representative axial, radial, and volumetric strain of the middle three layers of the specimen, respectively.