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Micro–macro properties of quartz sand: Experimental investigation and DEM simulation

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ABSTRACT

The ability to accurately simulate the realistic behavior of granular materials is one of the challenging issues of the numerical techniques. The first purpose of this study is to calibrate the microscopic properties of granular materials by Discrete Element Method (DEM). Coefficients of rolling and sliding friction as two main microscopic properties of granular material have a significant effect on the amount of macroscopic properties like Angle of Repose (AoR). Earlier studies indicated that the same AoR can be demonstrated by different combinations of the microscopic properties of materials. Therefore the AoR cannot singly be considered as a reliable criterion for DEM calibration, hence time as the second macroscopic property was considered along with the AoR for the calibration of microscopic properties. Furthermore, the need for further study in the field of fine particles led to the use of quartz sand with the diameter in the range of 300 to 600 μm in this study. It was assumed that the sand grains are spherical particles and dry material (non-cohesive).

In the first step of the calibration process, the Sandglass test was performed to measure the macroscopic properties of quartz sand. Then the Sandglass was simulated by DEM for a varied range of coefficients of rolling and sliding friction. A comparison between the AoR and discharging time of materials and DEM results indicated that the coefficients of rolling and sliding friction of sand particles are 0.3 and 0.52 respectively. The calibrated model was verified by performing a comparison between the experimental and simulation results of the conical pile test.

The second purpose of this research is to decrease the computational time of DEM simulation through utilizing a slice of a domain instead of the whole domain where the material slice represents the realistic mechanical behavior of materials. Therefore, a rectangular container was experimentally tested and numerically simulated at different thicknesses of the container. Both experimental and numerical results indicated that the critical thickness of the cabin is 32 times of the particle diameter at which the front and rear walls of the cabin do not restrict the mobility of particles in the median plane. In addition, when the wall boundary condition was replaced by periodic boundary condition, the critical thickness decreased to 4 times of particle diameter which significantly improved the computational speed.

1. Introduction

Granular materials are widely used in numerous industrial processes with a variety of forms and sizes, from large piece of iron ore to tiny grains of sand. Having a good understanding about the physical and mechanical properties of granular materials helps scientists and researchers to improve and optimize the quality of equipment and performance of industrial processes. Physical properties of materials are the measurable properties which describe the physical state of systems, such as density, color, shape, size, temperature, gravitation and velocity, whereas the mechanical properties are determined by measuring the reaction of material against a load (e.g. strength, toughness and ductility) [1].

The macroscopic properties (mechanical and physical properties) inherently depend on the microscopic properties of the materials. The macroscopic behavior of granular materials is determined not only by how discrete grains are arranged in space, but also by what kinds of interactions are operating among them [2,3]. Experimental approaches or numerical methods are conventional ways in determining the

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microscopic and macroscopic properties of granular materials. But since the microscopic parameters are only partially known, it is crucial and laborious to determine them by the experimental methods [3,4].

In the past decades, numerical techniques are utilized as a promising method in determining the microscopic properties of granular materials. Discrete Element Method (DEM) is a numerical technique that has been developed since 1971 [5]. The ability to accurately predict the granular flow makes DEM a popular choice of numerical techniques for many different applications.

The first issue with DEM is an accurate determination of the microscopic properties, e.g., spring stiffness, coefficients of friction, damping coefficients, bonding strength and coefficient of restitution. The microscopic properties should be specified such that the flow of thousands of particles behaves as same as the real granular material [6]. Therefore the macroscopic properties such Angle of Repose (AoR), bulk density, shear rate and material granulometry are utilized to find out the microscopic properties of granular material.

DEM is an expensive technique for modeling particulate systems at the individual particle scale. Number of particles, particle shape and particle size are some of the parameters that make DEM simulations expensive. Hence, some simplifications are inevitable and necessary. For instance, modeling the shape of a particle is computationally expensive with DEM, so rolling friction is often introduced in order to consider the shape effects [7]. In other words, the rolling friction is utilized to represent the effects of particle shape in the modeling of pseudo-static or dynamic systems of granular materials [8]. Consequently, the shape effect will be represented by the coefficient of rolling friction in this study.

Moreover, the AoR can be achieved by combining a wide range of coefficients of rolling and sliding friction [7,9]. Therefore, it is unavoidable to apply at least two independent macroscopic parameters in calibrating the microscopic properties. The amount of time an experiment takes is another macroscopic property that is applied as the second macroscopic property in this study to determine the microscopic parameters more accurate and reliable.

As already stated, the computational time is of high importance in DEM simulation and it depends on the physical properties of particle as well as the test condition [9–11]. It was indicated that the particle size is one of the main determinant items of computational time [12]. In other words, decreasing the particle size, increases the computational time and this is the reason that modeling the interaction of fine particles is expensive. One of the proposed methods for overcoming the expenses of particulate system modeling is utilizing a slice of the computational domain instead of the whole domain which represents the realistic mechanical behavior of the material. By this method, a substantial number of particles are not considered in DEM simulations and consequently the computational expenses decrease [13]. This idea is carried out through a container with two adjustable walls. It is clear that the front and rear walls of the container cause an additional restriction to limit the mobility of particles in contact with the walls [10]. Grasselli and Herrmann [14] did a series of experiments to determine the wall effect on the AoR. They utilized a different possible particle size ranging from 80 to 350 μm for powders and from 100 to 400 μm for glass spheres. Their experimental results illustrated that the critical container thickness where the walls do not have any effect on the AoR for the mentioned range of particle size is more than 100 times of particle diameter. Also Zhou et al. [10] observed that the critical value of container thickness for the coarse particles with the diameter in the order of 2–10 mm, is about 20 times of particle diameter.

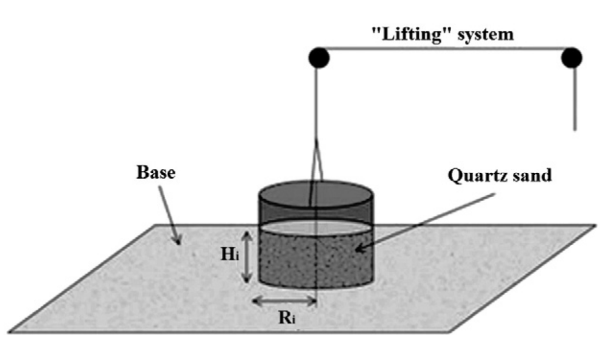

Fig. 1. Scheme of the experimental setup to determine the AoR in the conical pile test.

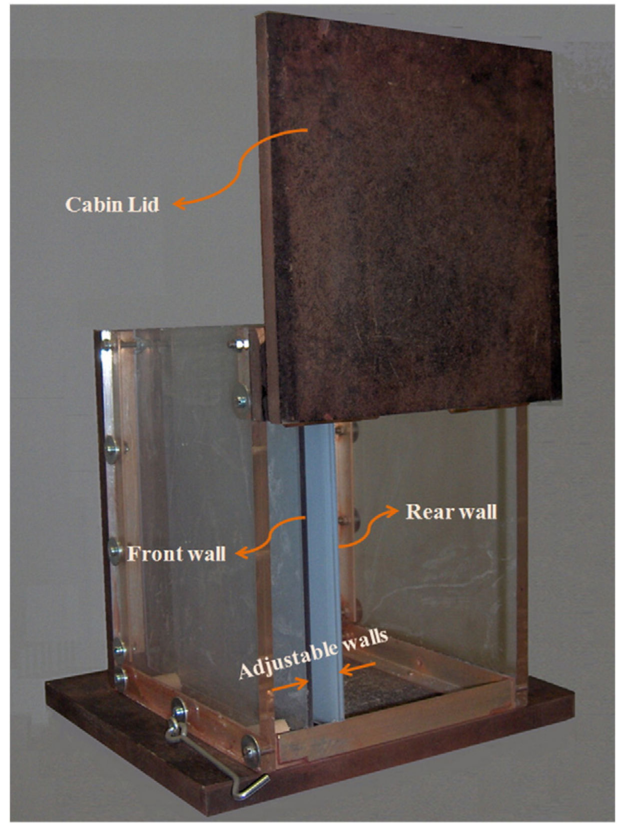

Fig. 2. Experimental setup of the rectangular container (sand particles are poured between the front and rear walls).

Numerous applications of the fine particles with the diameter in the range of 400 to 1000 μm, caused to use sand grains with the diameter in the range of 150 to 1000 μm in this study. Fine particles are classified in three groups based on the size distribution in micrometers: suspended atmospheric dust, settling dust and heavy dust [15]. In terms of particle size, these sand particles belong to the heavy dust subgroup with the diameter in the range of 100 to 1000 μm.

The objectives of this study are, first, extracting the microscopic properties of quartz sand through comparing experimental results and DEM results and, second, reducing the computational time of DEM simulation by using the smallest possible domain.

2. The framework of experiments

Various types of sand have a lot of applications in the industrial process and equipment. Hence, having an accurate and reliable determination about the physical and mechanical properties of sand is necessary because it helps scientists and researchers to improve and optimize the quality of equipment and performance of industrial processes.

In this study, quartz sand as the second most abundant mineral on the surface of earth is used in the experiments. In order to determine the physical properties of quartz sand, a series of experiments are conducted to obtain the particle density, bulk density and granulometry