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Investigation of the effective elastic parameters in the discrete element model of granular material by the triaxial compression test

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ABSTRACT

The general objective of the present paper is to improve the understanding of micromechanical mechanisms in granular materials and their representation in numerical models. Results of numerical investigations on micro–macro relationships in the discrete element model of granular material are presented. The macroscopic response is analysed in a series of simulations of the triaxial compression test. The numerical studies are focused on the influence of microscopic parameters on the initial response. The effect of the contact stiffness and friction coefficient on the effective elastic moduli is investigated. Numerical results are compared with the analytical estimations based on the kinematic Voigt's hypothesis as well as with selected numerical results of other authors. The comparisons show that a better agreement between the numerical and analytical results is observed for particle assemblies with higher coordination numbers. Higher coordination numbers are related to more compact specimens and for a given specimen can be associated with low values of the contact stiffness and a higher confining pressure.

1. Introduction

The discrete element method (DEM) proposed by Cundall and Strack [1] is a numerical procedure, in which a material is represented as a large assembly of rigid particles (discrete elements) interacting with each other by contact forces. It is a suitable tool to model materials with discontinuities. It has become a very popular framework to model granular materials in many applications in areas such as soil mechanics [2,3], geotechnics [4,5], agriculture [6,7], powder metallurgy [8] and others [9]. The DEM can also be used to model cohesive materials such as rocks [10,11] and concrete [12].

The discrete elements can be of spherical, e.g. [2,3,6], or non-spherical, e.g. [13,14], shape. In the present work, the spherical particles are used. The spherical geometry of the

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particle is idealized and does not accurately model phenomena exhibited by a real granular material. It has been shown that spherical particles give a smaller angle of repose and reduced shear strength as compared to non-spherical particles [13]. This is due to the fact that the rotation is only resisted by frictional contacts with neighbouring particles; whereas for non-spherical particles, the rotation tends to be inhibited by mechanical interlocking. The deficiencies of spherical particles can be mitigated to a certain degree by introducing the rotational friction in the contact model. It has been shown in [9], that the rotational friction increases the angle of repose. Including the rolling friction allows to reproduce properly macroscopic flow of a granular material [6]. Despite their deficiencies spherical particles are very popular in the DEM, e.g. [2,3], and are very often chosen for simulation mainly because of their low computational costs.

The discrete element model is a micromechanical material model. A required macroscopic behaviour is obtained taking an adequate contact model with appropriate parameters. The macroscopic response of a granular material is described by the deformability, strength, dilatancy, strain localization etc. The initial deformation is characterized by the elastic constants, i.e. Young's modulus, Poisson's ratio, bulk modulus and shear modulus. The discrete element model is defined in terms of microscopic parameters such as the interparticle contact stiffness parameters, damping coefficients, rolling and sliding friction. A simple contact model employing a linear law for the normal compressive force and the frictional Coulomb model for the tangential force has been used in this work.

Use of the discrete element model requires determination of the microscopic contact parameters. It is sometimes possible to measure material and contact properties of a single particle [6,7], but in most cases macroscopic tests and measurements on a granular material are available only. Then in order to determine the microscopic parameters the relationships between microscopic and macroscopic parameters must be established. Constitutive micro–macro relationships for discrete element models of granular materials can be obtained analytically or numerically.

In analytical approaches, based on micromechanical modelling and homogenization procedures, effective macroscopic properties are derived in terms of interparticle parameters and particle assembly properties, cf. [15–18]. Theoretical micromechanical approaches employ the kinematic hypothesis of uniform strain (Voigt's hypothesis), cf. [15–17] or the static hypothesis of uniform stress (Reuss hypothesis), cf. [19]. The Voigt's kinematic hypothesis leads to an upper bound solution for elastic moduli. Implementation of the static hypothesis for granular materials does not often strictly satisfy all the requirements of equilibrium and therefore lower estimation and not lower bound solution can be obtained, cf. [19].

Different simplifying assumptions are required in the microstructural analysis. Many formulations assume equal size particle assembly, cf. [20,21] or regular particle configuration, cf. [22–24]. Some of the above referenced works, cf. [15–17] employ the assumption that there is no sliding at contacts, thus they are applicable to small strain and elastic behaviour only. The microstructural constitutive relationship for granular systems has been extended in [25] to take into account the effect of particle separation and sliding under large deformation. The extension consisted in applying a standard homogenization procedure in an incremental way to a statistical representation of a granular material.

Numerical simulations are a useful tool to study micromechanical mechanisms in granular materials. Numerical investigation of elastic properties of granular packings has been presented in [26]. Micromechanical study of elastic moduli of two-dimensional granular assemblies using the DEM has also been carried out in [27,23]. Theoretical micromechanical predictions of effective moduli of identical spheres have been compared with numerical simulations in [21]. Comparisons of numerical and theoretical results show that in some cases, analytical estimation gives good results, cf. [23], but in many cases, discrepancy between analytical estimations and numerical results can be observed, cf. [28]. The discrepancy is caused by the lack of compatibility of the discrete element assembly characteristics with the simplifying assumptions of the theoretical homogenization. Therefore, analytical equations can be used for a preliminary estimation of the microscopic parameters, but numerical simulations are necessary in a more reliable calibration of the discrete element model.

The numerical calibration of a discrete element model of granular materials can be performed employing the computational homogenization approach [29,12] or by simulation of laboratory tests, such as the direct shear test [5,30,31], the repose angle test [9], or the triaxial compression test [3,32,33]. Microscopic parameters are determined by fitting numerical result to experimental one. A discrete element model of the triaxial compression test will be used in the numerical studies in the present work.

The investigation is focused on the initial response and elastic effective moduli of a granular material. The term "elastic" is used here in the sense adopted in an engineering practice for moduli measured in standard laboratory tests. Actually, the tangent moduli obtained from the slopes of respective experimental stress–strain curves are not "true elastic" since they are influenced not only by the elasticity of the material but also by irreversible effects caused by the friction and grain rearrangement [26].

The present work has been aimed to establish the relationships between the microscopic parameters and macroscopic properties of a granular material and to verify validity of the theoretical formulae for elastic moduli for a wide range of microscopic parameters influencing the elastic response. We have tried to fill the gap between the works aiming just to calibrate the model by matching numerical results to experimental ones and the works presenting micromechanical studies.

The elastic moduli obtained in numerical simulations will be compared with analytical estimations according to the Voigt's hypothesis. The closed-form expressions for the Voigt's bounds are obtained assuming only force interactions therefore in our simulations we will use the contact model taking into account the force interaction only, and neglecting the moment interaction due to the rolling friction. We are aware that by neglecting the rolling friction we impose some limitations on the range of possible macroscopic parameters [34], nevertheless, it is necessary to understand micromechanical mechanisms of this simple model before enriching it with other effects such as the moment interactions.