Investigation of micro-macro relationships of elastic parameters in the discrete element model of granular material

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Abstract

A general objective of the paper is to improve understanding of micromechanical mechanisms in granular materials and their representation in numerical models. Results of numerical investigation on micro-macro relationships in the discrete element model of granular material are presented. The macroscopic response was analysed in a series of simulations of the triaxial compression test. Numerical studies were focused on the influence of microscopic parameters on the elastic response. The effect of the contact stiffness and the contact stiffness ratio on the effective elastic moduli, the Young's modulus and Poisson's ratio, were investigated. Numerical results were compared with the analytical estimations.

Keywords: discrete element method, granular material, triaxial test, micro–macro relationship, Voigt hypothesis, elastic moduli

1. Introduction

The discrete element method (DEM) employing spherical particles became a very popular framework to model granular materials. In the DEM, a material is represented as a large collection of rigid particles (discrete elements) interacting with one another by contact forces. The discrete element model belongs to a class of micromechanical material models. Calibration of the discrete element models aiming to establish the relationship between microscopic and macroscopic model parameters is the key issue in an effective use of the discrete models to model real materials. Constitutive micro-macro relationships for discrete element models of granular materials can be obtained analytically or numerically.

In the present work, numerical simulations of the triaxial compression test will be performed aiming to establish the relationships between the microscopic parameters and macroscopic properties of a granular material. The investigation is focused on the initial response and elastic effective moduli of a granular material. Numerical results will be compared with analytical micro-macro relationships derived from the Voigt kinematic hypothesis.

2. Analytical micro-macro relationships

The Voigt hypothesis is based on the assumption that a particle assembly is subjected to a uniform strain state and the displacements of individual particles are in accordance with the displacement field induced by the uniform strain.

For an assembly of spherical particles of the same size and same material properties with isotropic packing structure, the closed-form formulae for the equivalent macroscopic Young's modulus E and Poisson's ratio ν can be derived in the following form [2, 3]:

$$E = \frac{n_c(1-e)k_n}{2\pi r} \cdot \frac{2k_n + 3k_t}{4k_n + k_t}, \quad \nu = \frac{k_n - k_t}{4k_n + k_t} \tag{1}$$

where n_c is the so-called coordination number, a parameter defined as an average number of contacts per particle, k_n and k_t are the contact stiffness in the normal and tangential direction, respectively, r is the particle radius, and e is the specimen porosity. The Voigt kinematic hypothesis leads to an upper bound solution for elastic moduli. It should be reminded that the above expressions are valid for the stick contact without sliding and without any moment-type interaction at the contact point.

3. Discrete element simulation results

Numerical simulations of the triaxial compression test were performed using a discrete element code DEMpack [1] for the cylindrical specimen shown in Fig. 1. The specimen is composed of 5,430 spherical particles with radii varying from $r_{\min} = 0.462$ mm to $r_{\max} = 0.89$ mm. The initial porosity of the specimen is $e = 0.39$. The particle mass density is equal to $\rho = 1660$ kg/m^3.

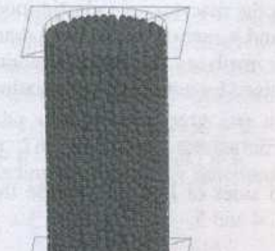

Figure 1: Discrete element model of the triaxial compression tests

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The granular material is modelled using the cohesionless contact model with sliding friction, neglecting a rolling resistance. The interparticle Coulomb friction coefficient $\mu = 0.5$ was assumed. The confining rigid walls were assumed nearly smooth with the Coulomb coefficient $\mu = 0.02$ for the particle–wall friction. The problem was studied for different values of micromechanical parameters: the contact stiffness k_n and the ratio of the contact stiffness in the tangential and normal directions k_t/k_n.

The results for different values of the contact stiffness k_n, the constant ratio $k_t/k_n = 0.35$ and the confining pressure 100 kPa are shown in Figs. 2 and 3 in the form of the curves showing the evolution of the deviatoric stress and volumetric strain, respectively, as functions of the axial strain.

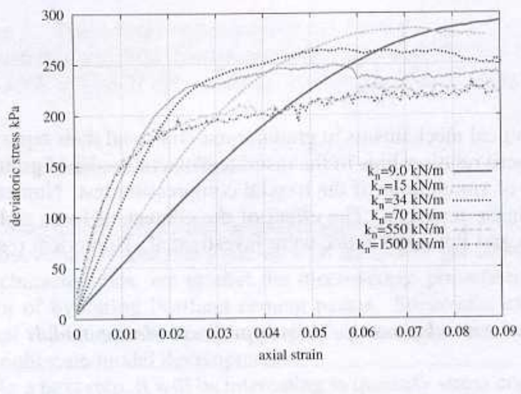

Figure 2: Deviatoric stress vs. axial strain for different values of the normal contact stiffness

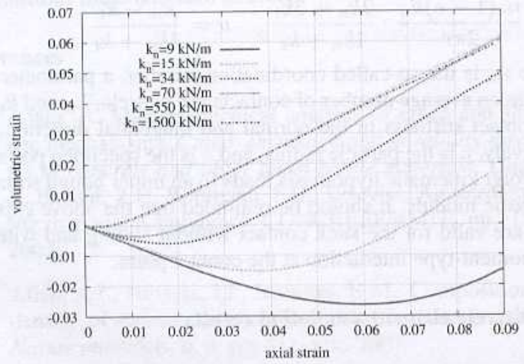

Figure 3: Volumetric strain vs. axial strain for different values of the normal contact stiffness

The elastic macroscopic parameters, the Young's modulus E and the Poisson's ratio ν, were determined from the initial slopes of the curves shown in Figs. 2 and 3. Dimensionless relationships involving the macroscopic elastic moduli and microscopic parameters k_t and k_n are plotted in Figs. 4 and 5. The dimensionless parameters involving the Young's modulus E and Poisson's ratio ν are obtained by rewriting the equations (1) as follows:

$$\frac{2\pi E r}{n_c(1-e)k_n} = \frac{2+3(k_t/k_n)}{4+(k_t/k_n)}, \quad \nu = \frac{1-(k_t/k_n)}{4+(k_t/k_n)} \tag{2}$$

The right-hand sides of Eqs. 2 provide theoretical predictions plotted in Figs. 4 and 5.

4. Conclusions

It can be seen that the numerical results are bounded by the theoretical predictions derived using the Voigt hypothesis. The lower is the contact stiffness k_n, the closer are the numerical results to the theoretical ones.

The analytical formulae for macroscopic elastic moduli are based on the assumption that there is no sliding at contacts, therefore the difference between the numerical and theoretical results is smaller for small values of the contact stiffness – the smaller the stiffness the bigger is the penetration of the particles and interparticle sliding and rearrangement play a minor role in an overall particle assembly deformation.

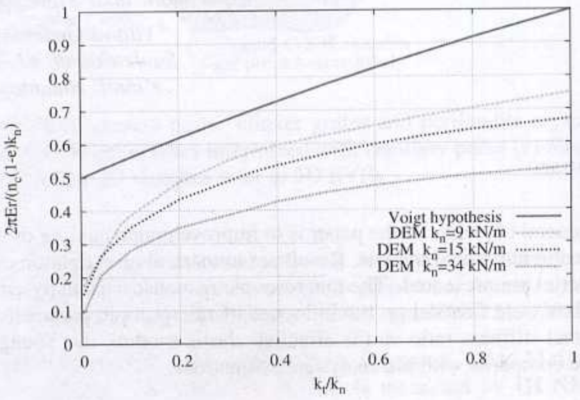

Figure 4: Analytical and numerical dimensionless relationships involving the Young's modulus as functions of the ratio k_t/k_n

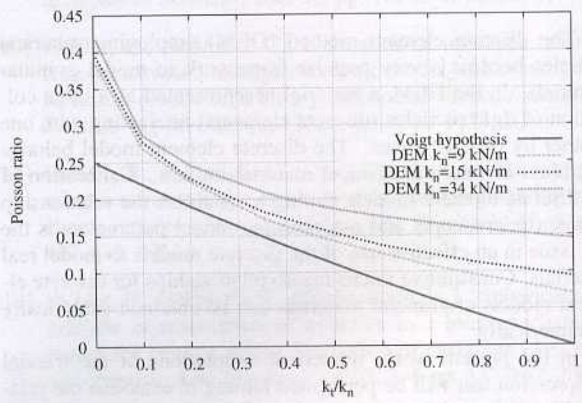

Figure 5: Poisson's ratio as a function of the ratio k_t/k_n – comparison of numerical and analytical relationships

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