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The impact of porosity and crack density on the elasticity, strength and friction of cohesive granular materials: Insights from DEM modelling

Martin P.J. Schöpfer [a,*], Steffen Abe [b,1], Conrad Childs [a], John J. Walsh [a]

[a] Fault Analysis Group, UCD School of Geological Sciences, University College Dublin, Belfield, Dublin 4, Ireland
[b] Seismology & Computational Rock Physics Laboratory, UCD School of Geological Sciences, University College Dublin, Belfield, Dublin 4, Ireland

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ABSTRACT

This study uses the Discrete Element Method (DEM), in which rock is represented by bonded, spherical particles, to investigate the dependence of elasticity, strength and friction angle on porosity and crack density. A series of confined triaxial extension and compression tests were performed on samples that were generated with different particle packing methods, characterised by differing particle size distributions and porosities, and with different proportions of pre-existing cracks, or uncemented particle contacts, modelled as non-bonded contacts. The 3D DEM model results demonstrate that the friction angle decreases (almost) linearly with increasing porosity, and is independent of particle size distribution. Young's modulus, strength and the ratio of unconfined compressive strength to tensile strength (UCS/T) also decrease with increasing porosity, whereas Poisson's ratio is (almost) porosity independent. The pre-eminent control on UCS/T is, however, the proportion of bonded contacts, suggesting that UCS/T increases with increasing crack density. Young's modulus and strength decrease, while Poisson's ratio increases with increasing crack density. The modelling results replicate a wide range of empirical relationships observed in rocks and underpin improved methods for the calibration of DEM model materials.

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1. Introduction

Knowledge of the mechanical properties of rocks is fundamental for both Earth scientists and engineers. Failure envelopes and elastic parameters are crucial for modelling a wide range of geomechanical problems, including wellbore failure, slope stabilities and the stability of underground excavations [1]. Rock properties are obtained from in situ tests and more commonly in the laboratory from samples that are loaded using stress and/or displacement controlled experiments. These tests have given many insights into the behaviour of rock and have shown, for example, that the elastic parameters and strength depend on porosity and cement content, though the details of these dependencies are also partly controlled by mineral composition (e.g., carbonate vs. siliciclastic rocks; [2,3]). Obtaining core samples from depth for laboratory testing is both time-consuming and expensive. Hence, rock physical properties are often estimated using empirical relations, such as the correlation between Young's modulus and sonic velocity, or that between unconfined compressive strength (UCS) and porosity [4]. Rock is, however, a heterogeneous material and even multiple samples obtained from a single slab of rock can exhibit significant variability in composition and hence mechanical behaviour [3]. Therefore, some of the above mentioned empirical rock property relations are poorly constrained. One of the principal aims of this work is to investigate these empirical property relations in numerical rock analogues where the effects of compositional heterogeneity can be isolated.

Numerical modelling offers a new avenue to better understand material property relations. An advantage of numerical modelling is that the user can examine systematically the effect of varying individual input parameters while keeping all other parameters constant; this is rarely possible with laboratory measurement. The Discrete Element Method (DEM), where rock is represented as an assemblage of particles (spheres, ellipsoids, blocks) that interact with each other, is ideal for investigating mechanical property relations since the user predefines microproperties (particle and cement properties) and determines macroproperties (elastic and strength parameters) using numerical lab experiments [5]. The mechanical behaviour of the model material is not predefined, as in continuum approaches, but emerges from the interaction of particles and cement [6].

The aim of this study is to investigate the impact of particle size distribution (PSD), porosity and cement content

* Corresponding author. Tel.: +353 17162611; fax: +353 17162607.
E-mail address: martin@fag.ucd.ie (M.P.J. Schöpfer).
[1] Present address: Geologie-Endogene Dynamik, RWTH Aachen University, Aachen, Germany.

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(i.e., proportion of bonded contacts) on the mechanical properties (elasticity, strength, ratio of unconfined compressive strength to tensile strength (UCS/T) and friction angle) of DEM model materials in 3D. In Section 2, we provide a brief review of rock property relations which are relevant for this study. In later sections, we describe the results of the various numerical mechanical experiments conducted on samples generated using a range of different packing methods and compare the observed failure envelopes, failure criteria and mechanical property relations (cement content, porosity) with those of rocks. This paper is concerned with defining relations between different mechanical properties rather than reproducing the behaviour of particular natural rocks: the numerical material properties in this study overlap with, but can also go well beyond, those of natural rocks. Neither have we explored the micromechanical origins of the observed mechanical property relationships. Calibration to the mechanical properties of particular natural rocks and investigation of related fundamental micromechanical issues are the subject of ongoing research.

2. Rock property relations and failure envelopes

In this study, we numerically investigate relations between porosity, cement content and rock mechanical properties. Here, we summarise the most important empirical relations obtained from lab experiments (see Fig. 1), which provide the essential backdrop to the numerical modelling presented in Section 4.

Probably, the most commonly used failure criterion for rock is the Coulomb criterion, which, expressed in terms of the principal stresses σ_1 and σ_3 ($\sigma_1 > \sigma_3$ and compressive stresses positive throughout this paper), is written as

$$\sigma_1 = \mathrm{UCS} + \sigma_3 \tan^2\left(45^\circ + \frac{\varphi_i}{2}\right), \quad (1)$$

where UCS is the unconfined compressive strength and φ_i is the angle of internal friction, the tangent of which is called the coefficient of internal friction μ_i [1]. Experimental data and theoretical models [7] suggest, however, that a linear failure criterion is only valid over a limited range of confining pressures and that a non-linear failure envelope concave towards the minimum principal stress axis (in a σ_1 vs. σ_3 plot) may prove to be the rule rather the exception [2]. An additional limitation of both linear and non-linear failure criteria is that they are often independent of the intermediate principal stress, σ_2 (Mohr criteria), whereas data from polyaxial tests suggest that many rock types exhibit a σ_2-dependence of strength [3,8]. Consequently, peak stress data and associated failure envelopes obtained from triaxial extension and triaxial compression tests exhibit a mismatch, where the former plots above the latter in a σ_1 vs. σ_3 plot (Fig. 1a). Under some circumstances, this mismatch can be eliminated by using a criterion that takes the impact of σ_2 into account (Fig. 1b). Finally, very few experimental data exist within the tensile field ($\sigma_3 < 0$; Fig. 1a) to define the transition from tensile to shear failure [9], though a parabolic failure envelope is most commonly used [10].

Laboratory tests of rocks indicate that strength, angle of internal friction and Young's modulus decrease with increasing porosity ([4,11–14]; Figs. 1c–e). Additionally, the presence of pre-existing cracks, which have been simulated in the laboratory by cyclically heating the rock specimen before loading [15,16], has a significant impact on rock mechanical properties (Figs. 1f–h). For example, strength and Young's modulus decrease whereas UCS/T increases with increasing number of heating cycles, changes which can be attributed to increases in the proportion of non-cohesive grain–grain contacts or crack density.

3. Methods

3.1. Discrete Element Method

The results in this paper have been obtained using two different 3D implementations of the DEM for spherical particles, the Particle Flow Code (PFC3D; [5,17]) and ESyS-Particle (formerly LSMearth; [18,19]). Both codes implement a linear force–displacement contact law with Coulomb friction and a particle–particle bond model that transmits both force and moment. The majority of the results presented in this paper were obtained using PFC3D and the microproperties used are given in Table 1. The details of the contact and bond law implementation are slightly different in ESyS-Particle, hence only UCS/T values are given and compared to those obtained from PFC3D.

As stated earlier, in a DEM model microproperties are defined and the macroproperties are obtained using numerical lab experiments, details of which are given in Section 3.3. The user therefore varies the microproperties systematically until the material exhibits the desired macroscopic mechanical behaviour. There are, however, two problems with calibrating DEM models consisting of spherical particles to match the response of real rock: (i) The (internal) friction angle of both cohesive and non-cohesive materials is typically too low, irrespective of the contact (i.e., particle–particle) friction coefficient [20]. Previous attempts to increase the friction angle have included modifications to the standard DEM approach including the use of clumped [5,21,22] or elliptical particles [23], implementing a rolling resistance [24] and explicitly prescribing the macroscopic failure criterion using hybrid methods [25]. (ii) UCS/T of DEM models of cohesive rock is too low (ca. 3–4) compared to rock (>10), an issue that has only recently been addressed in 2D [22,26]. We show later that both the low friction angles and low UCS/T values obtained in previous studies were partly a consequence of the particle packing methods used, which lead to porosities that were too high to achieve realistic properties without modifying the standard DEM. In this study, we show that different particle packing methods, and hence different PSD and model porosity, combined with different proportions of bonded contacts can replicate the range of friction angles and UCS/T values associated with rocks.

3.2. Model generation and packing methods

There are two end-member methods for generating random dense packing of spheres for DEM simulations, constructive and dynamic [27]. For this study, we used one constructive method, the particle insertion method [28], and one dynamic method, the specimen genesis procedure widely used by PFC3D users [5] (Fig. 2).

The dynamic specimen genesis procedure used for this study, which is described in detail in Ref. [5], is based on a four-step process: (i) Particles with radii chosen randomly from a uniform size distribution are randomly generated within a volume bound by planar, frictionless walls. (ii) The system is allowed to adjust by particle movement under zero friction. (iii) A low isotropic stress is installed by modifying the radii of all particles simultaneously. (iv) The radii of particles that have less than three contacts are modified iteratively, so that these particles have at least three contacts (over 99% of particles have four or more contacts in the final model) and their mean contact normal force is low in relation to the mean contact force of the assembly. Models generated with the dynamic method had a uniform PSD with r_{max}/r_{min} of 1.66 (Fig. 3) and a porosity of ~37% (model (i) in Fig. 2).

For the particle insertion method, 'seed' particles are first generated within the specimen domain. The specimen is then

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