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A discrete element model predicting the strength of ballast stones

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ABSTRACT

An extended discrete element method (DEM) is used to describe strength and failure properties of ballast stones. For this purpose, a rock material is modeled using spherical particles bonded by breakable force elements. An inflation procedure to generate dense sphere packings which is based on a particle's current coordination number is proposed. The particle bonds are enhanced by a progressive failure model that reproduces the effects of singular stress concentrations near crack tips, which are normally not present in DEM, by successive weakening of bonds. The material model is investigated in uni- and triaxial compression, where an efficient approach for the simulation of a flexible confining membrane is applied, and calibrated to granite yielding wide agreement in strength and failure properties. Furthermore, a procedure to model shape and angularity of ballast particles is proposed. Finally, the strength of ballast stones made from bonded particles is subjected to statistical evaluation and compared to published experimental results. Different measures for single particle strength are investigated with respect to the loading state which causes failure.

1. Introduction

One very important area of application of the discrete element method (DEM) is in the field of geomechanics [1,2] where the method originated [3]. The DEM can be extended to the simulation of breakable materials by introduction of particle bonds. This approach is particularly advantageous for materials such as rocks, which themselves are granular on micro-scale, since often no adequate continuum descriptions of deformation and especially failure exist. Furthermore, the fracture of bonded particulate matter inherently reproduces many effects of the failure process of this kind of materials.

Discrete element methods using bonded particles have extensively been used to study problems involving fracture or disintegration of rock, see e.g. [4–7]. In [8] a comparison between different simulative approaches to this kind of problems is performed. The failure of particle bonds was related to acoustic emission measurements in [9]. The problem of parameter calibration was addressed in e.g. [10].

Bonded particle DEM was also applied to investigate the behavior of ballast. Fracture is considered within the context of simplified ballast particle shapes or breakable asperities [11–13]. The simulation of realistically shaped ballast was up to now restricted to unbreakable stones [14–16].

In this research an implementation of the DEM in the simulation package Pasimodo [17] is used to study the failure of geomaterials, i.e. strong rock and ballast. Firstly, the bonded particle model is described. As dense particle packings are required to produce strong materials, a procedure is proposed to generate sphere packings, that feature a significantly higher average coordination number than standard approaches. Therefore, a particle's current coordination number is used as a control variable for an inflation procedure.

Then, the bonding concept and a progressive failure model based on damage accumulation are introduced. The progressive failure model reduces the strength of the remaining bonds at particles, which have already been involved in bond breakage, in order to promote brittle, localized fracture and reproduce the effects of singular stress concentrations near crack tips that are intrinsically not present in DEM. The material model is calibrated to granite by simulation of uniaxial compression tests. Strength and failure in uniaxial and triaxial compression are investigated in detail. An efficient model of the stress boundary condition in triaxial tests is implemented.

Finally, a procedure to extract realistically shaped angular ballast stones from the granular solid is proposed. Using several tangent planes on ellipsoids of matching size the angular shape of ballast particles can be reproduced reasonably well. This novel approach allows creating breakable, irregularly shaped stones for further simulative investigation. The crushing strength of stones created in this way is statistically evaluated and failure mechanisms and measures of strength are discussed.

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2. Granular solid from bonded particles

The DEM was developed for the simulation of systems consisting of distinct rock blocks [3]. Its general concept can be applied to any system of particles of arbitrary shape, where the system behavior is governed by the interaction of these particles on a mesoscopic scale. Usually contact forces are obtained from penalty approaches that avoid particle overlap. Thus, they can be, but do not need to be, based on physical laws. A simple and common approach to describe the interaction force F_{ij} in normal direction of particles i and j is a linear spring-damper combination

$$F_{ij} = k_{ij}\delta_{ij} + d\dot{\delta}_{ij} \tag{1}$$

with stiffness and damping constants k_{ij} and d, respectively. For spherical particles the overlap δ_{ij} is related directly to the particle positions $\boldsymbol{x}$ and radii r by $\delta_{ij} = r_i + r_j - \|\boldsymbol{x}_i - \boldsymbol{x}_j\|$ and the contact force is only applied if $\delta_{ij} > 0$.

The stiffness constant can be calculated based on the idea of an elastic rod (Young's modulus E) between the centres of the particles

$$k_{ij} = \frac{EA_{ij}}{L_{ij}} = \frac{E\pi r_{ij}^2}{2r_{ij}} = \frac{\pi}{2}Er_{ij}, \tag{2}$$

whose cross section A_{ij} and length L_{ij} depend on the average radius $r_{ij} = \frac{1}{2}(r_i + r_j)$. Thus, the idea of an elastic rod introduces some physical motivation into the penalty approach. The damping constant can be related to the dimensionless damping ratio, see [18] for more details.

The DEM can be extended to the simulation of granular solids by introducing bilateral particle bonds that generate forces even in case of negative overlap, i.e. a gap, between two bonded particles. A granular solid is generally created by bonding adjacent particles from a dense packing. Fracture and failure phenomena can be incorporated in these models by removal or weakening of bonds based on suitable failure criteria. The advantage of this approach is that multiple fractures at arbitrary locations of the solid may happen and no initiation of cracks is necessary. The crack path is only limited by the discretization, i.e. fracture occurs on the level of bonds between unbreakable particles. For sufficiently small particles this states no serious limitation. Bond breakage based on the loading condition and system dynamics causes cracks to propagate, bifurcate or coagulate.

2.1. Generation of dense sphere packings

The generation of a suitable initial configuration is the first step of every DEM simulation. In case of simulations dealing with bonded particles this initial configuration is a dense packing of particles that are to be bonded. A variety of approaches exists for the generation of such a packing, see e.g. [19] and references therein.

A homogeneous and isotropic sphere packing can be obtained by continuously reducing the ratio $\psi = l/2\bar{r}$, where $\bar{r}$ denotes the average particle radius and l is a characteristic length of the domain containing the particles. This can be achieved by either compression of the volume containing the particles or inflation of the particles inside of a fixed domain. In both cases a dilute initial configuration of non-overlapping particles has to provided, which can be obtained from regular lattices that might be randomly disturbed.

Inflation schemes usually employ a radii growth rate $\dot{R}$ which is equal for all particles at one instant in time. In most general form, this scheme reads

$$\dot{r}(t)/r(t) = \dot{R}(t). \tag{3}$$

The normalized growth rate $\dot{R}$ might be constant or time dependent.

It is proposed, to modify this scheme by introducing a dependency of a particle's individual normalized growth rate on its coordination number c_n

$$\dot{r}(t)/r(t) = \max(\dot{R}[1 - c_n(t)/\hat{c}_n], 0), \tag{4}$$

where $\hat{c}_n$ denotes a "desired" coordination number that serves as a further control parameter for the inflation procedure. The intention of this modification is to increase the average coordination number $\bar{c}_n$ while keeping particle overlap small. As long as the system is dilute, i.e. $\bar{c}_n \ll 1$, the scheme corresponds to Eq. (3). When a particle's coordination number rises, this particle's growth rate is reduced. Hence, particles with a smaller coordination number will grow faster than particles with a higher one. This leads to a significantly higher average coordination number. Shrinkage of particles is prohibited, which allows for the use of a desired coordination number $\hat{c}_n$ that is smaller than the maximal coordination numbers of all particles. This is important, as the effect of the modified scheme decreases when $\hat{c}_n$ is increased. In the limit case of $\hat{c}_n \to \infty$ Eq. (4) reduces to Eq. (3). On the other hand, if $\hat{c}_n$ is chosen too small, no sufficient compaction is achieved.

Obviously, this scheme may lead to a distortion of the particle size distribution. The amount of distortion depends directly on $\hat{c}_n$. Smaller $\hat{c}_n$ result in a stronger effect on particle size distribution. Usually, the radii distribution is only affected slightly, but clearly, if a well defined radii distribution after compaction is required the scheme cannot be applied. Fig. 1(a) shows particle size distribution curves before and after coordination based inflation. It can be seen, that the radii of the smaller particles are increased more than those of the larger ones. The larger particles are likely to have a higher number of contacts in an earlier stage of inflation due to their size, whereas the smaller particles may grow with a higher rate. Generally, this trend increases as $\hat{c}_n$ is reduced. Nevertheless, the width of the distribution remains nearly unaffected.

The development of the average coordination number is compared in Fig. 1(b) for the standard and modified scheme. It is apparent that from a pressure above $p \approx 2$ MPa the average coordination number is significantly higher with the modified scheme. Final values are $\bar{c}_n = 6.6$ for the modified and $\bar{c}_n = 6.0$ for the standard scheme. The latter being the well known number for a random packing of monodisperse spheres. Pressure is used here as a simple external measure for stored deformation energy or average overlap of the spheres, as they are directly related by the stiffness of the interactions. Hence, the developed coordination number based inflation scheme yields a sphere packing with a significantly higher average coordination number.

It was realized that during inflation it might be favorable to use soft interactions of the spheres with the boundary walls of the domain for two reasons. Firstly, packings generated with softer walls show a higher average coordination number. Secondly, layering of particles near the walls is reduced, as significant overlap of a number of particles and the walls may develop. The effect of particle layering is discussed in [18].

2.2. Bonding concept

Particle bonds usually correspond to force laws which act in restricting at least one degree of freedom of the relative motion of the bonded particles. In this study, the bonds are limited to the normal direction, and are represented by springs that act between the centres of the bonded particles. Shear, bending and twisting is not inhibited [20,21]. The model used here employs either a bond or a repulsive contact interaction. The contact force results from the bond as long as it is intact. For particles that are not or no longer bonded a repulsive interaction is applied.