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CONSTITUTIVE RELATIONS OF DENSE GRANULATES WITH FRICTION AND ADHESION FROM DEM

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Summary. Granular materials in a split-bottom ring shear cell geometry show wide shear bands under slow, quasi-static deformation. From discrete element simulations (DEM), continuum fields like the deformation gradient and stress can be computed with the goal to formulate objective constitutive relations for the flow behavior. From a single simulation only, by applying time- and (local) space-averaging, yield loci can be obtained: linear for non-cohesive granular materials and non-linear with peculiar pressure dependence for adhesive powders.

1 INTRODUCTION

Discrete Element Models (DEM) allow the specification of particle properties and interaction laws and then the numerical solution of Newton's equations of motion [1, 2]. For geotechnical applications and industrial design in mechanical engineering, one of the main challenges is to obtain continuum constitutive relations and their relevant parameters from experimental and numerical tests on representative samples.

DEM simulations of similar element tests provide advantages with respect to physical experiments, as they provide more detailed information of forces and displacements at the grain scale. Finding the connection between the micromechanical properties and the macroscopic behavior involves the so-called micro-macro transition [3–8]. Extensive "microscopic" simulations of many homogeneous small samples, i.e., so-called representative volume elements (RVE), have been used to derive the macroscopic constitutive relations needed to describe the material within the framework of a continuum theory [3, 5].

An alternative – as presented in this study – is to simulate an inhomogeneous geometry where static packings co-exist with dynamic, flowing zones and, respectively, high density co-exists with dilated zones. From adequate local averaging over equivalent volumes – inside which all particles behave similarly – one can obtain from a single simulation already constitutive relations in a certain parameter range, as was done systematically in two-dimensional (2D) Couette ring shear cells [6, 9] and three-dimensional (3D) split-bottom ring shear cells [8, 10].

The special property of the split-bottom ring shear cell is the fact that the shear band is initiated at the bottom gap between the moving, outer and fixed, inner part of the bottom-wall. The velocity field is well approximated by an error-function [7, 8, 11, 12] with a width considerably increasing from bottom to top (free surface). The data-analysis provides datasets of different pressures, shear-stresses and shear-rates – from a single simulation only. Previous simulations with dry particles were validated by experimental data and quantitative agreement was found with deviations as small as 10 per-cent [8, 10, 12]. Note that both time- and space-averaging are required to obtain a reasonable statistics. Furthermore, we remark, that even though ring-symmetry and time-continuity are assumed for the averaging, this is not true in general, since the granular material shows non-affine deformations and intermittent behavior. Nevertheless, the time- and space-averages are performed as a first step to obtain continuum quantities – eaving an analysis of their fluctuations to future studies.

The DEM simulation is based on peculiar contact models as described in Refs. [13, 14], where we use the elasto-plastic-adhesive frictional model as detailed in Ref. [13]. This model is used in the split-bottom geometry as introduced in Refs. [11, 15, 16] experimentally, and examined by DEM simulations without cohesion in Refs. [8, 10]. More details can be found in these references – here we just present the yield loci for different cohesion strength.

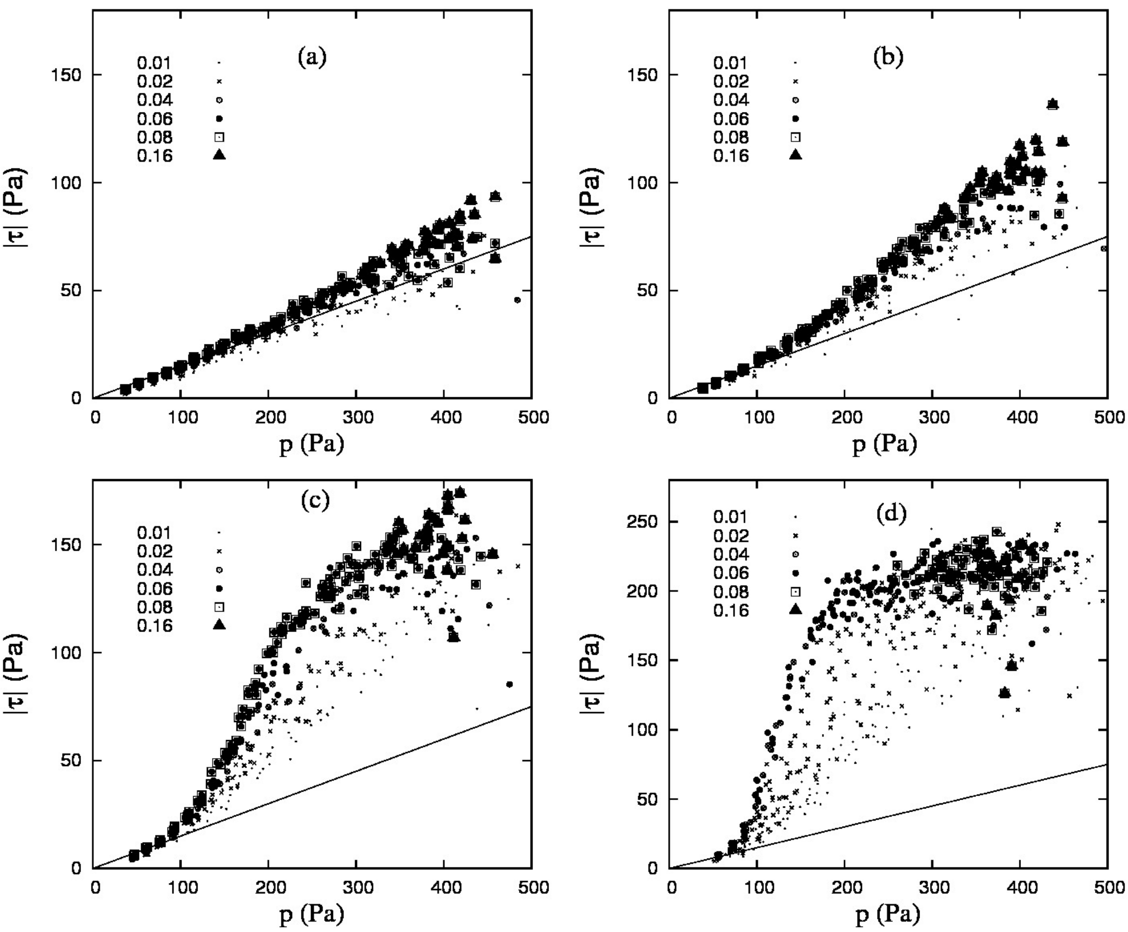

Figure 1: Shear stress plotted against normal stress (yield locus) for different contact adhesion strengths 0, 1/10, 1/5, and 2/5. The solid line represents the yield locus for frictionless material with linear normal force.

2 RESULTS

While frictionless and frictional spherical granular matter shows yield loci that are almost linear [8, 10], with slopes around ~0.15 and ~0.3, respectively, the behavior in the presence of contact adhesion is much less predictable as discussed below. When contact adhesion is included in the model, a non-linear yield locus is obtained with peculiar pressure dependence. This non-linearity becomes apparent when plotting the shear stress against pressure for different coefficients of adhesion, as shown in Fig. 1. The main effect of contact adhesion is to increase the strength of the material under large confining stress. For weak adhesion the strength is given by an almost linear relation between shear stress and pressure, while the relation is highly non-linear for large adhesion.

The microscopic reason of this nonlinearity is the non-linearity of the contact model: The contacts feel small adhesion forces for small experienced pressure (close to the free surface). Very large adhesion forces are active for high pressures deep in the bulk of the material. Therefore the micromechanical mechanisms involve not only plastic deformation of the contact zone, but also sintering, fragmentation and re-bonding under large stress conditions.

3 CONCLUSIONS

Simulations of a split-bottom Couette ring shear cell with dry granular materials show perfect qualitative and good quantitative agreement with experiments. The effect of friction was studied recently, so that in this study the effect of contact adhesion was examined in some detail. The yield locus, i.e., the maximal shear stress, plotted against pressure – for those parts of the system that have experienced considerable shear (displacement) – is almost linear in the absence of adhesion, corresponding to a linear Mohr-Coulomb type yield locus with slope (macroscopic friction) increasing with microscopic contact friction.

Strong non-linearity of the yield locus emerges as a consequence of the strong adhesive forces that increase non-linearly with the confining pressure. Due to the non-linearity, the definition of a macroscopic cohesion (as shear stress of the yield locus at zero-stress) becomes questionable. All this interesting phenomenology is due to the history dependent contact model: Contacts that experienced large stresses can provide much larger adhesive forces than others which have not been compressed a lot. Therefore, at the top (free surface) the yield stress is much lower then deep inside the sample.

The physical origin of this nonlinearity is the permanent deformation at the contact which leads to a larger contact surface area and therefore to stronger van der Waals forces. As final remark, we note that the model contains an unphysical simplification: The long range van der Waals adhesion is neglected and only the short range contact adhesion is considered. Future studies with the long range (non-contact) term will show whether this can lead to more linear and cohesive yield locus. In real systems of dry, adhesive powders, the long range adhesion will provide the bulk cohesion, since – as shown in this study – the contact adhesion alone is not effective at small confining pressure.

Future research will also involve the yield locus of materials with different friction, rolling resistance and torsion resistance.

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