FLOW BEHAVIOR OF AN-ISOTROPIC GRANULAR FLUIDS

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Summary Dense granular media are examined in 2D and 3D with molecular dynamics simulations. From various flow boundary conditions, an intrinsic an-isotropy of the packing is evidenced. The question of a constitutive model for dense, an-isotropic granular (shear) flow is attacked by means of a micro-macro transition aimed at macroscopic quantities like strain-, stress-, and material tensors. Results are presented for steady state flow in average over many snapshots at different times; time-series are used in non-steady situations.

INTRODUCTION

The flow behavior of dense powders is studied, using the discrete element method (DEM). Powders are typically inhomogeneous, non-linear, disordered, and an-isotropic on a "microscopic" scale [1], where the typical microscopic size is the particle size. An irregular random packing responds to a deformation via inhomogeneous and an-isotropic rearrangements and stress-response. Before the peak, one has softening, and beyond weakening is obtained, which is typical for over-consolidated powders. Besides an experimental verification of the simulation results [2], the formulation of constitutive relations in the framework of continuum theory is the great challenge. One promising material model for dry sand is the so-called hypoplastic theory [3], for which the material parameters can be determined either experimentally, or from DEM simulations, as shown in this study. The elementary units of granular materials are "mesoscopic" grains that locally, at the contact point, deform under stress. Since the realistic modeling of the deformations of the particles is much too complicated, the interaction force is related to the overlap Δ of two particles. Two particles interact only if they are in contact, and the force between these two particles is decomposed into a normal and a tangential part. For the sake of simplicity, we restrict ourselves to spherical particles here. The normal force is, in the simplest case, a linear spring that takes care of repulsion, and a linear dashpot that accounts for dissipation during contact. The tangential force involves dissipation due to Coulomb friction, but also some tangential elasticity that allows for stick-slip behavior on the contact level [2,4]. If all forces acting on a selected spherical particle (either from other particles, from boundaries or from external forces) are known, the problem is reduced to the integration of Newton's equations of motion for the translation and rotational degrees of freedom. The simulations with the discrete element model [4] use a two-dimensional bi-axial box, where the left and bottom walls are fixed. Stress- or strain-controlled deformation is applied to the side- and top-walls, respectively.

RESULTS

The system examined in the following contains N=1950 particles with radii randomly drawn from a homogeneous distribution with minimum 0.5 mm and maximum 1.5 mm [4]. The friction coefficient used in the two-dimensional simulations is μ=0.5. In Fig. 1 (left), the volume change of a typical simulation indicates, first, compression, then dilatancy, and eventually a very weak change at large deformations (up to 20 per-cent). At the same time, the stress response, in Fig. 1 (right) (where the indices xx and zz denote horizontal and vertical stresses, respectively), shows elastic, softening, and critical state flow behavior.

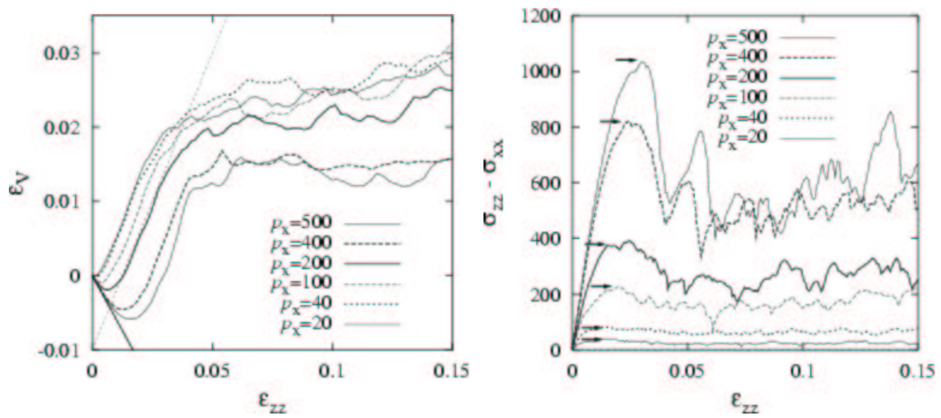

Figure 1: Volumetric strains (left) and stresses (right) during large deformations, both plotted against vertical strain, for different side pressures p_x, as indicated in the inset. The peak yield stress is marked by the arrows in the right plot.

First, the vertical stress increases linearly; then the slope gradually decreases (softening), until the stress reaches its maximum (peak yield stress). After the peak, further softening/weakening behavior (with negative slope) is followed by a constant, strongly fluctuating stress for larger deformations.

From the simulation data presented in Fig. 3, it is possible to obtain the following material parameters, as based on an isotropy assumption: The initial slope (-0.59) of the volumetric strain determines the Poisson ratio; the slope of the volumetric strain in the dilatancy regime (0.80) is related to the dilatancy angle; the initial slope of the stress is related to the initial bulk modulus, and the peak (yield) stress is related to the flow function of the material, as detailed in the following. It is possible to examine the flow behavior of the system by plotting Mohr-circles for the maximum stress (right-most point on the circle) for different confining pressures (left-most point), see Fig. 2. The eigen-directions of the system are parallel to the walls, because there is no friction active between particles and walls, so that the left- and right-most points on the circles are indeed corresponding to the wall stresses; note that in an arbitrary geometry, it is not necessarily that simple. The tangent to the circles (slope 0.588) can be seen as the flow function for peak stress. It is linear for the examined parameters, with its slope only slightly larger than expected from the microscopic friction at the contacts alone. Since we have not used cohesive forces, the macroscopic cohesion c is non-existent, i.e., the flow function hits the origin.

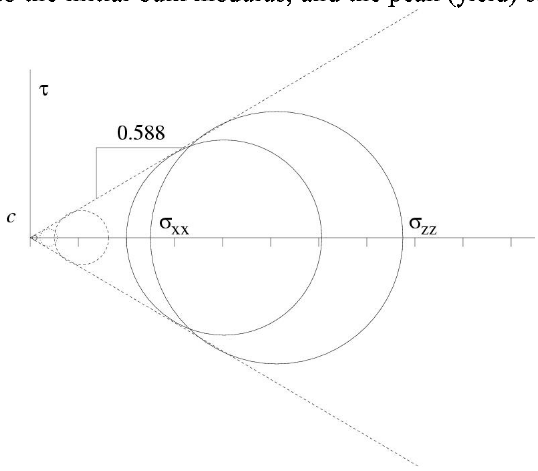

Figure 2: Mohr circle representation of the flow function at peak stress, see the arrows in Fig. 1 (right).

HYPOPLASTIC MATERIAL PARAMETERS

Some of the material parameters involved in a hypoplastic material theory [3] can also be extracted from these simulation data. An essential ingredient of the theory is the functional behavior of the pore number: $e^h = e_0^h \exp\left(-\left[p/h_s\right]^n\right)$, as a function of the pressure. The empirical model parameters for this function (based on experimental findings) involve the pore number at vanishing stress, e_0^h, the so-called granular hardness, h_s, and an empirical power n. This is astonishingly close to the fit-function for the initial and the critical state pore-number envelope, see Fig. 3, $e(e_0,n) = e_0 - \left[p/h_s\right]^n$, where the parameters e_0 and n can be read off from the inset, and the granular hardness was set equal to the spring stiffness $h_s = 10^5$ in the DEM contact model. Both expressions can be related to each other via a series expansion in the small variable p/h_s.

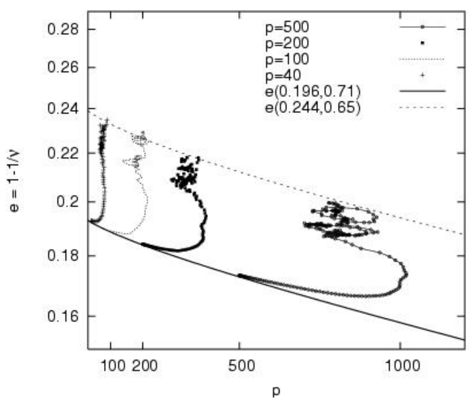

Figure 3: Pore number plotted against side stress for different confining pressures – data are taken from the simulations in Fig.1.

SUMMARY AND CONCLUSIONS

A set of DEM simulations in a bi-axial box configuration was presented, and several macroscopic material parameters were extracted from the data. Besides the an-isotropic material response, the behavior of the density (pore-number) as function of the confining pressure was discussed and related to a hypoplastic material law [3]. This is a first step towards a micro modeling approach for cohesive frictional powders. Further material parameters have to be identified, and also the effect of cohesion has to be examined more closely, in both 2D and 3D. Also the role of particle rotations (active in the shear-band) is an open issue, as related to micro-polar constitutive models.

Acknowledgements: This work was funded by FOM, NL and the DFG, Germany; furthermore, helpful and inspiring discussions with H.-J. Butt, M. Kappl, M.-K. Müller, K. Nübel, R. Pitchumani, J. Tejchman, J. Tomas, and R. Tykhoniuk are acknowledged.

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