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ScienceDirect
Particuology 6 (2008) 501–505
PARTICUOLOGY
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Constitutive relations for the shear band evolution in granular matter under large strain

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Received 31 May 2007; accepted 15 July 2008

Abstract

A so-called “split-bottom ring shear cell” leads to wide shear bands under slow, quasi-static deformation. Unlike normal cylindrical Couette shear cells or rheometers, the bottom plate is split such that the outer part of it can move with the outer wall, while the other part (inner disk) is immobile. From discrete element simulations (DEM), several continuum fields like the density, velocity, deformation gradient and stress are computed and evaluated with the goal to formulate objective constitutive relations for the powder flow behavior. From a single simulation, by applying time- and (local) space-averaging, a non-linear yield surface is obtained with peculiar stress dependence.

The anisotropy is always smaller than the macroscopic friction coefficient. However, the lower bound of anisotropy increases with the strain rate, approaching the maximum according to a stretched exponential with a specific rate that is consistent with a shear path of about one particle diameter.

Keywords: Ring shear cell; Shear bands; DEM simulation; Micro–macro transition; Objective constitutive relations; Yield stress fluid

1. Introduction

Granular matter consists of many independent particles with peculiar collective flow behavior. Knowing the interaction laws and inserting those into a discrete element model (DEM), one can follow the particles by integrating Newton’s equations of motion (Herrmann, Hovi, & Luding, 1998; Kishino, 2001; Luding, 2004b, 2008b; Luding, Lätzel, & Herrmann, 2001).

One goal is to derive continuum constitutive relations – as needed for industrial application. Methods and tools for a so-called micro–macro transition are applied (Lätzel, Luding, & Herrmann, 2000; Luding, 2004a, 2005a, 2005b, 2008b; Vermeer et al., 2001) on small so-called representative volume elements (RVE). In ring shear cells, both local space averaging (on toroidal sub-volumes at fixed radial and vertical position) as well as time-averaging in the (presumed) steady state can be applied. One obtains already from a single simulation some of the constitutive relations aimed for. Here, the micro–macro averaging is applied to a three-dimensional split-bottom ring shear cell as recently introduced (Fenistein & van Hecke, 2003; Fenistein, van de Meent, & van Hecke, 2004). The special property of a split-bottom ring shear cell is the fact that the shear band is initiated at the bottom slit and its velocity field is well approximated by an error-function (Fenistein et al., 2004; Luding, 2004b, 2006) with a width considerably increasing from bottom to top (free surface). In this study, the frictionless data are examined closer and the stress- and strain-tensors are studied in their eigensystems and eigen-directions. A recently proposed evolution equation for the deviatoric stress (Luding, 2008c) is examined.

2. The soft particle molecular dynamics method

The behavior of granular media can be simulated with the DEM (Allen & Tildesley, 1987; Lätzel, Luding, Herrmann, Howell, & Behringer, 2003; Luding, 2008a). As the basic ingredient, a force-displacement relation that governs the interaction between pairs of particles is defined. Particle positions, velocities and interaction forces are then sufficient to integrate (explicitly) Newton’s equations of motion and follow all particles during the evolution of the system under large strains.

Since the modeling of the internal deformations of the particles is much too complicated, we relate the normal interaction force to the overlap as $f = k\delta$, with a stiffness k, if $\delta > 0$. In order to

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doi:10.1016/j.partic.2008.07.020

Nomenclature

r, ϕ, z	radial [m], angular [rad] and vertical coordinates [m]
f	contact force [N]
k	contact stiffness [N/m]
δ	contact deformation (overlap) [m]
μ	contact friction coefficient
μ_{macro}, ψ	macroscopic friction coefficient and friction angle [rad]
R_{o}, R_{s}, R_i	outer wall-, slit-, and inner wall-radius [m]
R_{c}, W	center and width of the shearband [m]
f_o, Ω_{o}	rotation rate [1/s] and angular frequency [1/s] of the outer wall
υ_ϕ, $\dot{\gamma}$	angular velocity [m/s] and strain rate [1/s]
I	non-dimensional strain rate
l_γ	shear path [m]
$\hat{\gamma}$	eigenvector perpendicular to the shear plane
θ	tilt of $\hat{\gamma}$ from the horizontal [rad]
$\sigma_{\alpha\beta}$	static stress tensor components [N/m^2]
$\sigma_{\max}$, σ_0, $\sigma_{\min}$	eigenvalues of the stress tensor [N/m^2]
$\hat{\sigma}_{\max}$, $\hat{\sigma}_0$, $\hat{\sigma}_{\min}$	eigenvectors of the stress tensor
$\lvert\tau\rvert$, σ_{D}	shear and deviator stress magnitude [N/m^2]
ρ	[kg/m^3]

account for energy dissipation, the normal degrees of freedom, i.e., the relative motion of two particles in contact, is subject to a viscous, velocity dependent damping, for more details see Luding (1998, 2008a).

3. Split-bottom ring shear cell

In order to save computing time, only a quarter of the ring-shaped geometry is simulated, using quarter periodic boundary conditions in angular direction. (In top-view, a particle that leaves the quarter system downwards, enters at the same radial position from the right – with according, unchanged velocity in cylindrical coordinates.) The walls are cylindrical, and are roughened due to some (about 3% of the total number) attached particles (Luding, 2004b, 2006, 2008b, 2008c). The outer cylinder wall with radius $R_{\mathrm{o}} = 0.110$ m, and part of the bottom $r > R_{\mathrm{s}} = 0.085$ m are rotating around the symmetry axis with the same rotation rate, while the inner wall with radius $R_{\mathrm{i}} = 0.0147$ m, and the attached bottom-disk $r < R_{\mathrm{s}}$ remain at rest.

First, the simulation runs for more than 50 s with a rotation rate $f_{\mathrm{o}} = 0.01\ \mathrm{s}^{-1}$ of the outer cylinder, with angular velocity $\Omega_{\mathrm{o}} = 2\pi f_{\mathrm{o}}$. For the average only larger times are taken into account, thus disregarding the transient behavior at the onset of shear. Two snapshots (with and without friction) are displayed in Fig. 1.

Translational invariance is assumed in the tangential ϕ-direction, and averaging is thus performed over toroidal volumina over many snapshots in time (typically 40–60), leading to fields $Q(r, z)$ as function of the radial and vertical positions. Here, averaging is performed with spacings of $\Delta r \approx 0.0025$ m and $\Delta r \approx 0.0028$ m in radial and vertical direction. The choice of these spacings is arbitrary, since they do not affect the results discussed below if varied somewhat. However, much smaller spacing leads to bad statistics and stronger fluctuations while much larger spacing leads to poor resolution and thus loss of information.

The averaged data from simulations lead to density, coordination number, and the isotropic fabric, all decreasing with height and systematically lower in the shear band due to dilatancy. From a set of simulations with different filling heights (data not shown, see Luding, 2004b), just examined from the top (like in the original experiments), it becomes clear that the shear band moves inwards with increasing filling height and also becomes wider. From the front-view, the same information can be evidenced, see Fig. 1, as well as shear band shape and width inside the bulk. The shear band moves rapidly inwards deep in system – close to the slit in the bottom – while its position does not change much further up.

4. Velocity gradient and stress tensors

From the velocity field gradient, the strain rate

$$\dot{\gamma} = \sqrt{d_1^2 + d_2^2} = \frac{1}{2}\sqrt{\left(\frac{\partial \upsilon_\phi}{\partial r} - \frac{\upsilon_\phi}{r}\right)^2 + \left(\frac{\partial \upsilon_\phi}{\partial z}\right)^2}, \tag{1}$$

is obtained, see Fig. 2, as discussed in Depken, van Saarloos, and van Hecke (2006), see Eq. (7) therein, where the geometrical term, υ_ϕ / r in Eq. (1), comes from the cylindrical coordinate system. From the eigenvalue analysis of the velocity gradient, one finds that shear planes are well described by the normal unit vector $\hat{\gamma} = (\cos\theta, 0, \sin\theta)$, with $\theta = \theta(r, z) = \arccos(d_1/\dot{\gamma})$, as predicted in Depken et al. (2006). This unit vector, $\hat{\gamma}$, is the eigenvector of the vanishing eigenvalue of the velocity gradient tensor, while the other two are opposite-equal, with their eigenvectors in the plane perpendicular to $\hat{\gamma}$ and both tilted by 45° from the r–z-plane. From the simulation, one can determine the components of the static stress tensor

$$\sigma_{\alpha\beta} = \frac{1}{V}\sum_{c \in V} f_\alpha l_\beta, \tag{2}$$

with the contact normal forces f_α and branch vector l_β components. The sum includes contacts in the vicinity of the averaging volume, V, weighted according to their vicinity.

Since the σ_{rz} component is small ($\sigma_{rz} \approx 0$), as compared to the other averaged non-diagonal stresses, the shear stress can be defined in analogy to the velocity gradient, as proposed in Depken et al. (2006):

$$|\tau| = \sqrt{\sigma_{r\phi}^2 + \sigma_{z\phi}^2}. \tag{3}$$

A more detailed study of the stress- and strain-eigenvalues and eigensystems leads to the three eigenvalues $\sigma_{\max}$, σ_0, and $\sigma_{\min}$ corresponding to the maximum, intermediate and minimum stress, respectively, with corresponding eigen-directions $\hat{\sigma}_{\max}$, $\hat{\sigma}_0$, and $\hat{\sigma}_{\min}$. In Fig. 3, the shear stress $|\tau|$ and the deviator stress