2D cyclic pure shear of granular materials, simulations and model

D. Krijgsman and S. Luding

Multi Scale Mechanics, Universiteit Twente, Faculty of Engineering Technology, MESA+, P.O. Box 217, 7500 AE Enschede, The Netherlands

Abstract. Discrete particle simulations of granular materials under 2D, isochoric, cyclic pure shear have been performed and are compared to a recently developed constitutive model involving a deviatoric yield stress, dilatant stresses and structural anisotropy. The original model shows the cyclic response qualitatively, but suffers from an artificial drift in pressure. With a small modification in the definition of the stress anisotropy and an additional limit-pressure term in the evolution equation for the pressure, it is able to show the transient as well as the limit cycles. The overall goal – beyond the scope of the present study – is to develop a local constitutive model that is able to predict real life, large scale granular systems.

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INTRODUCTION

Dense granular materials are widely encountered in industrial processes, such as hopper discharge, chute flow and fluidized beds. Grains in these materials interact with multiple neighbours for finite durations and stress is largely transmitted through force chains. Due to the disordered behaviour of these particles, the materials show peculiar mechanical properties quite different from classical fluids or solids, like dilatancy, yield stress, history dependence and anisotropy. The Discrete Particle Method (DPM), in which the forces on each particle are calculated and integrated over a finite time, is able to capture all of these properties, however has the major drawback that it is computationally too expensive for realistic, large scale systems.

Constitutive models are an option to simulate real problems instead of just laboratory scale experiments with. Many of such models have been developed in literature [1, 2, 3, 4], which all have their own advantages and disadvantages. In this work a further look is given to the model proposed and applied to cycling loading by Magnanimo and Luding [5, 6]. Besides equations for the stresses, the model also incorporates an evolution equation for the anisotropy, which allows it to predict dilatancy, yield stresses, cope with the history dependent nature of the material, and provide anisotropic material properties.

Simulations are performed by the DPM package Mercury [7] and are used to calibrated the model, both in the original form and the modified version.

CONSTITUTIVE MODEL

In this section a short overview of the used constitutive model is given. For more information the reader is referred to the original work [5, 6]. The local model starts from the incremental Hooke's law:

$$\delta\sigma_{ij} = C_{ijkl}\delta\varepsilon_{kl} \tag{1}$$

From there it assumes that in the bi-axial box system, the stress and strain tensors only have diagonal components, such that they can easily be split into volumetric and deviatoric parts, leading to:

$$\begin{bmatrix} \delta\sigma^h \\ \delta\tau \end{bmatrix} = \begin{bmatrix} 2B & A \\ A & 2G \end{bmatrix} \begin{bmatrix} \delta\varepsilon^v \\ \delta\gamma \end{bmatrix} \tag{2}$$

Now it is the goal to find expressions for the bulk modules B, the shear modulus G and the anisotropy modulus A. Two basic modifications of the elastic model with constant moduli are in, a non-linear stress evolution (with yield stress) and a varying anisotropy, while initially B and G are assumed constant. In this paper a third additional modification is proposed called the pressure stabilization.

Non-linear stress evolution

From DEM simulations it has been widely observed that for increasing shear strains, the stress increments decrease until the stress saturates in the critical state regime. This is modelled by multiplying the incremental shear strain with the stress anisotropy S:

$$\begin{bmatrix} \delta\sigma^h \\ \delta\tau \end{bmatrix} = \begin{bmatrix} 2B & A \\ A & 2G \end{bmatrix} \begin{bmatrix} \delta\varepsilon^v \\ S\delta\gamma \end{bmatrix} \tag{3}$$

with

$$S = 1 - \frac{\tau}{\sigma^h} \frac{\mathrm{sign}(\delta\gamma)}{s^d_{max}} \quad (4)$$

where $s^d_{max} = \left(\frac{\tau}{\sigma^h}\right)_{max}$ is the absolute maximum allowable deviatoric stress ratio in the material after long shear deformation.

Varying anisotropy

The second modification is to prescribe the anisotropy modulus as an evolution equation dependent on the shear strain:

$$\frac{dA}{d\gamma} = \beta_A \left(A_{max} - \mathrm{sign}(\delta\gamma) A\right) \quad (5)$$

with A_{max} the absolute maximum allowable anisotropy in the material and β_A a parameter that determines how fast the anisotropy changes and thus how fast saturation is approached. If $\delta\gamma$ does not change sign, equation (5) can be solved analytically:

$$A = \mathrm{sign}(\delta\gamma) A_{max} \left(1 - e^{-\beta_A|\gamma|}\right) + e^{-\beta_A|\gamma|} A_0 \quad (6)$$

with A_0 the initial anisotropy at $\gamma = 0$.

Pressure stabilization

On top of these two features a new pressure stabilization term is proposed. The goal of this term is to stabilize the model for shear cycles (otherwise the pressure would continuously in/decrease), as well as to provide a better model for the transient leading to the limit cycles. The term is a simple addition to the differential pressure equation in the form of:

$$\beta_p \left(\sigma^h_{steady}(\phi) - \sigma^h\right) |\delta\gamma| \quad (7)$$

where β_p is a rate parameter and $\sigma^h_{steady}(\phi)$ is the expected steady state pressure dependent on the packing fraction. In this paper, however, only one packing fraction is studied, so the dependence on the packing fraction is omitted.

SIMULATIONS

The results from the model are compared with DPM simulations. These simulations are performed by the DPM package Mercury [7], which integrates Newtons equations of motion for a large number of particles based on a velocity Verlet algorithm. The forces are due to interactions between particles (modelled as a visco-elastic normal force) and a much smaller background friction:

$$m\ddot{\vec{x}}_i = \vec{f}_i = \gamma_b \dot{\vec{x}}_i + \sum_{i \neq j} \left(k\delta_{ij} + \gamma_p \dot{\delta}_{ij}\right) \vec{n}_{ij} \quad (8)$$

TABLE 1. Simulation parameters and material model

Parameter	Value	Explanation
k	10000 Nm^{-1}	Contact stiffness
γ_p	0.2938 Nsm^{-1}	Inter particle viscosity
γ_b	0.0294 Nsm^{-1}	Background friction
ρ	20 kgm^{-3}	Particle density
Δt	$1.3 \cdot 10^{-5}$ s	Simulation time step
t_c	$6.5 - 13 \cdot 10^{-4}$ s	Collision time
r_n	$0.80 - 0.89$	Coefficient of restitution

where γ_b is the background friction, $\vec{x}_i$ the location of particle i, k the contact stiffness, δ_{ij} the overlap between particles i and j, γ_p the inter particle viscosity and $\vec{n}_{ij}$ the normal vector pointing from particle j to i. The parameters used in this study are shown in table 1. To remove the effect of walls on the simulation, both boundaries are modelled as periodic walls.

Initial conditions

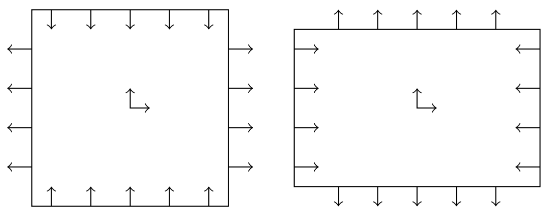
The initial packing is prepared by inserting 10 000 particles with a homogeneous size distribution ($r^{min} = 3.7 \cdot 10^{-3}$ m and $r^{max} = 7.4 \cdot 10^{-3}$ m) at random positions (with small random velocities) in a large square domain. Then the system is slowly compressed to the desired packing fraction, $\phi = 0.85$, where it equilibrates until the kinetic energy has decayed to very small values.

Simulation details

During the simulation the particles are subjected to pure shear cycles (see figure 1). Pure shear is induced by moving the two periodic walls while conserving the volume. The walls move slowly according to a cosine profile, until a maximum shear strain of $\gamma = 0.001$. After it has reached its maximum strain amplitude, the shear direction is reversed and the simulation continues until the original shape of the box is retained at the end of each cycle. One complete cycle takes $4 \cdot 10^6$ time steps and the ratio of kinetic to potential energy is always small ($E_k/E_p < 0.002$). Therefore, it is assumed that the system is in the quasi-static, shear rate independent regime. Note that, even though size and shape of the box, at the start and at the end of the simulation, are the same, the stress and anisotropy states can differ dramatically.

RESULTS

In the DPM simulations an initial transient is clearly visible until after about 100 cycles. From there on the system is in a state where limit cycles are present (see the pressure variation in figure 3). First the limit cycles are discussed and later the transient.



(a) Initially $(\delta\gamma > 0)$ (b) Going back $(\delta\gamma < 0)$

FIGURE 1. Deformation mode

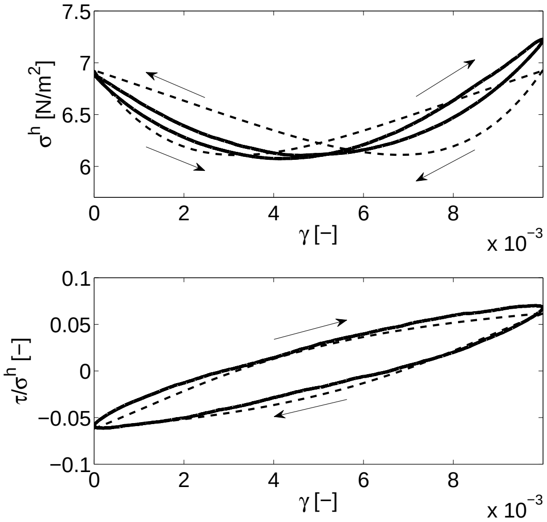


FIGURE 2. Evolution of pressure, and the shear stress over pressure ratio during a cycle after 200 cycles. Arrows indicate the direction of shear; for a more clear picture averages are taken over the last 50 cycles. Solid curves are averages of the simulation results and the dashed curves lines are a fit using the model (both the improved as the original model show the same behaviour)

Limit cycles

The evolution of the pressure and the shear stress over pressure ratio, during a shear cycle in the limit cycle state, are shown in figure 2. Here the stress curves form closed loops, meaning that the stress state at the start and at the end of a cycle are equal. At the start of each cycle more of the contacts between particles will be aligned in the compressive direction of the previous half-cycle, giving rise to the structural anisotropy and the corresponding anisotropy modulus A (data not shown). At each strain reversal, the contacts in the previously dominant direction will become weaker or even open, resulting in a drop of anisotropy and pressure and an increase in shear stress. As the simulation continues, the smaller fraction of contacts in the shear compression direction will become stronger and new contacts can form. Halfway through the first half of the cycle, loosening and strengthening of contacts are in equilibrium, resulting in a roughly constant pressure, whereas the shear stress continues to increase. Near the end of first half-cycle, the slope of the shear stress curve starts to decrease, meaning that the system is starting to saturate. If one would continue to shear in the same direction, finally the pressure would also saturate. In the second half-cycle the system will experience a similar opening and closing of contacts, but with exchanged directions, until it returns to its initial state.

The model is qualitatively able to reproduce the simulations. All of the three phases discussed before show the correct behaviour. However, two distinct differences are visible: First, the locations of the minima in the pressure; in the simulations the minimum pressure is almost in the symmetry (centre) point, whereas the model shows two minima, closer to the shear reversals. Secondly, the model suffers from a tiny but significant drift in pressure. To be able to produce limit cycles (i.e. the variables having the same value at the start end at the end of each cycle) the model has to be symmetric around the average deformation, which is achieved by the correction term in equation (7).

Isotropic stress saturation

The need for an additional term also shows up if one does not only look at the last (stable) cycles, but also at the approach to this state. The evolution of the pressure is shown as a function of the number of cycles for 4 different simulations in figure 3. Due to the isotropic preparation phase the initial packings have a high pressure. During the shear cycles the particles wiggle around and can find more efficient configurations, resulting in less overlap and a significantly reduced pressure. As more cycles are simulated the pressure at the start of each cycle saturates at roughly 6.5 Nm^{-2}.

To search for the instability of the model and to be able to obtain stable limit cycles, the model is analytically examined in the limit of small pressure variations around an average pressure (note that this is not the case in the simulation results). In this limiting case the same pressure is used as in the pressure stabilization term (σ^h_{steady}), so that equation (4) simplifies to:

$$S = 1 - \frac{\tau}{\sigma^h_{steady}} \frac{\mathrm{sign}\,(\delta\gamma)}{s^d_{max}} \qquad (9)$$

which makes the whole set of equations analytically solvable, resulting in:

$$\sigma^h = C_1 + A_{max}\left(\frac{4}{\xi+\beta_A} e^{-(\xi+\beta_A)\gamma} - \frac{2}{\xi} e^{-\xi\gamma}\right) \qquad (10)$$

$$\tau = \sigma^h_0 s^d_{max}\left(1 - C_2 e^{-\gamma\xi}\right) \qquad (11)$$

TABLE 2. Parameter values and initial conditions used for the model as shown in figure 2 and 3. The initial conditions of the improved model are the same as used in the simulations, starting from an isotropic initial state. The initial conditions for the original model are different since the model predicts the behaviour only in the limit cycle regime

Parameter	Original Model	Improved model	Explanation
G	51.5 Nm^{-2}	51.5 Nm^{-2}	Shear modulus
s^d_{max}	0.097	0.097	Maximal deviatoric stress ratio
A_{max}	593 Nm^{-2}	593 Nm^{-2}	Maximum anisotropy
β_A	159	ξ (Eq. (12))	Anisotropy growth factor
β_P	n.a.	2.5	Pressure growth factor
σ^h_{steady}	n.a.	6.3 Nm^{-2}	Steady state pressure
σ^h_0	6.93 Nm^{-2}	25 Nm^{-2}	Initial pressure
τ_0	-0.227 Nm^{-2}	0 Nm^{-2}	Initial deviatoric stress
A_0	403 Nm^{-2}	0 Nm^{-2}	Initial anisotropy

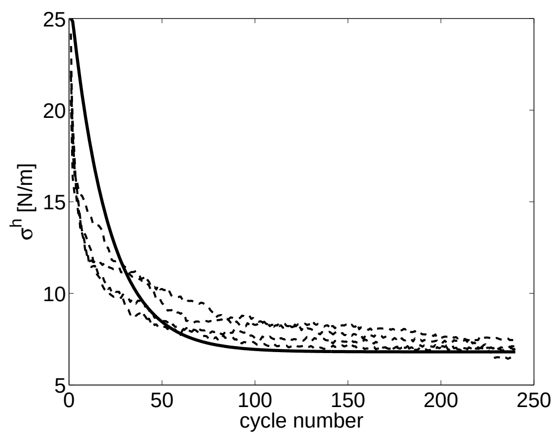


FIGURE 3. Evolution of the pressure at the start of a each cycle ($\gamma = 0$). Dashed curves show result for 4 different simulations, the solid curve shows results of the improved model.

with $\xi = 2G/\sigma^h_{steady} s^d_{max}$. To obtain limit cycles the pressure at the start and the end of the cycle have be be equal, while the shear stress should have changed sign. For simplicity we assume shear cycles with an infinite amplitude.

$$\begin{aligned} \sigma^h(0) &= \sigma^h(\infty) \qquad & \xi &= \beta_A \\ \tau(0) &= -\tau(\infty) \qquad & C_2 &= 2 \end{aligned} \tag{12}$$

How to interpret equations (12) is still an ongoing research, but in this paper β_A has been removed as a free variable. The results of the improved model can be seen in figures 2 and 3.

CONCLUSION

In this paper DPM simulations of granular materials under 2D, isochoric, cyclic pure shear have been compared to a recently proposed constitutive model. Originally the model is able to show the limit cycles qualitatively, but was unable to model the transient and suffered from a drift in pressure. With a small modification in the definition of the stress anisotropy and an additional term in the evolution equation for the pressure it predicts the transient as well as the limit cycles.

Further research will be performed on the influence of the magnitude of the shear strain, the packing fraction and the initial preparation procedure. Recent research [8] also suggests that the symmetry of the shear cycles is relevant for the stress state, especially during the first few cycles, an issue to be studied in more detail.

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