Simulating pressure-induced compaction by grain rearrangement

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This article presents a novel model of the compaction of loose sand, or other granular material, incorporating two dilatancy terms. One is negative, reflecting the general tendency of an assembly to collapse under a combination of shear stress and pressure. The other develops during shear straining and, at the critical state, is sufficiently large and positive to counter the negative contribution. The existence of a term producing negative dilatancy, however, suggests the concept of ‘self-cancelling shear deformation’. These shears contribute to the shear–volume coupling, producing densification, but not to the macroscopic shear deformation. They only occur when there is a small amount of damage. This produces pressure-induced densification by granule rearrangement, resulting in a model where compaction is possible under a hydrostatic load but the model can still simulate cyclic deformation and critical state behaviour.

KEYWORDS: compaction; constitutive relations; friction; numerical modelling; plasticity; sands

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INTRODUCTION

The densification of granular materials is important in a wide range of situations: from repairing pot-holes in roads to pill making and from the liquefaction of sands and silts during an earthquake to the slow consolidation of clay sediments. The mechanisms involved include crushing or plastically deforming the grains under pressure (Vesic & Clough, 1968; Coop, 1990), rearranging undamaged grains into a denser packing by slow cyclic deformation (Youd, 1972) or a combination of both. The authors are not aware of any models of granular materials that explicitly include both rearrangement and particle damage in a way that allows both mechanisms to interact. This article presents such a model.

The model building scheme utilised in its development facilitates the incorporation of micromechanical concepts into the macroscopic constitutive description of the granular assembly. This process, described in detail elsewhere (Chandler, 1985; Chandler & Sands, 2007a, 2010), starts with a kinematic constraint and dissipation function and produces appropriate flow rules and yield functions. This article focuses on a mechanism, called ‘self-cancelling shear strains’, whereby compaction of loose granular assemblies can be produced by hydrostatic pressure alone.

MODEL BUILDING SCHEME

Consider a unit volume of sand, in a Cartesian coordinate system x_1 , x_2 and x_3 , supporting macroscopic components of effective stress σ_{ij} and undergoing macroscopic components of strain e_{ij} . The convention of ‘tension positive’ is used throughout this paper for both stress and strain. Using the Einstein summation convention, it is convenient to define a mean effective stress $\sigma = \sigma_{mm}/3$ and a volume strain $e = e_{mm}$. It follows that the effective pressure is $-\sigma$. A dot over a symbol indicates a rate, or increment, and the volumetric strain rate ($\dot{e}$) is split into the part associated with particle rearrangement ($\dot{e}^R$) and that associated with

particle damage caused by direct affine compression across the contacts ($\dot{e}^D$), such that $\dot{e} = \dot{e}^D + \dot{e}^R$. In addition, deviatoric components of stress and strain are defined as

$$s_{ij} = \sigma_{ij} - \sigma \delta_{ij} \quad (1)$$

and

$$d_{ij} = e_{ij} - e \delta_{ij}/3 \quad (2)$$

where δ_{ij} is the Kronecker delta. The rate of doing work on the sand ($\dot{w}$) can then be written as

$$\dot{w} \equiv s_{ij} \dot{d}_{ij}^R + \sigma (\dot{e}^R + \dot{e}^D) \quad (3)$$

assuming, for the sake of simplicity, that most of the deviatoric strain rate occurs as a result of particle rearrangement and that affine sliding of particles is negligible (affine sliding of particles could, however, be taken into account as has been done elsewhere (Chandler et al. (2008)).

For the rigid plastic idealisation, an energy balance can then be written as

$$s_{ij} \dot{d}_{ij}^R + \sigma (\dot{e}^R + \dot{e}^D) - \dot{D}(\sigma, \dot{d}_{ij}^R, \dot{e}^D) = 0 \quad (4)$$

where $\dot{D}$ is the rate of dissipation. For thermodynamic consistency, this function is always positive and, to ensure the strain rate independence typical of sands, is always homogeneous of degree one in the strain rate components.

INCORPORATION OF SELF-CANCELLING SHEAR STRAINS

Imagine that, in addition to the macroscopic deviatoric strains d_{ij} , there might be shear strains at particle level that contribute to the dilatancy and to the dissipation rate but cancel each other out when averaged over a much larger volume. These therefore produce no net macroscopic shear strains. The rate of these, which we call self-cancelling shear strains, is denoted by the scalar $\dot{\alpha}$.

The pressure-dependent isotropic dissipation function used by Chandler (1990) and Chandler et al. (2008) is now extended to include the energy dissipated by direct compression and the self-cancelling shear strains, such that

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$$\dot{D} \equiv [\mu^2 \sigma^2 \dot{d}_{mn}^R \dot{d}_{mn}^R + k^2 \dot{\alpha}^2 + \ell^2 (\dot{e}^D)^2]^{1/2} \quad (5) \quad \text{and}$$

The parameter ℓ reflects the resistance to crushing at the contacts associated with direct volumetric affine compression, while k reflects the resistance to the damage occurring during particle rearrangement. Both have units of stress.

As $\dot{\alpha}$ is a variable akin to strain rate, it can be included in the dilatancy rule. A sophisticated dilatancy rule presented elsewhere (Chandler & Sands, 2007b) is extended for use in this model, such that

$$\dot{e}^R = v_i (\dot{d}_{mn}^R \dot{d}_{mn}^R + \dot{\alpha}^2)^{1/2} + 2v_r d_{ij}^g \dot{d}_{ij}^R \quad (6)$$

The first term on the right-hand side of equation (6) takes account of the tendency of a loose granular assembly to continually densify in response to granule rearrangement until a maximum density is achieved. It follows that v_i is always negative. The second term includes a positive parameter (v_r) and a governing strain ($d_{ij}^g = d_{ij}^R - d_{ij}^{\text{ref}}$, which allows for the influence of the recent strain history on subsequent behaviour) and takes account of the tendency of a moderately dense granular assembly to dilate in response to monotonically applied shear stress and immediately collapse on reversal of load. Together, the terms including v_i and v_r produce the volume changes associated with small cyclic shear strains and large monotonic shear strain (Sands & Chandler, 2011) and predict non-coaxiality of shear stress and shear strain rate when the principal axes rotate (Chandler & Sands, 2007b). In order to do this, v_i and v_r are constructed as functions of the current density and evolve as deformation progresses. The reference strain d_{ij}^{ref} holds the recent strain history and is defined by the differential equation

$$\dot{d}_{ij}^{\text{ref}} = c_1 d_{ij}^g (\dot{d}_{mn}^R \dot{d}_{mn}^R)^{1/2} \quad (7)$$

where c_1 is assumed to be a material constant (Chandler & Sands, 2007b). The parameters ℓ , k , v_i and v_r evolve as deformation progresses. The ratio ℓ/k is kept constant while ℓ , which is positive, evolves in accordance with

$$\ell = \ell_0 \left(\exp \left(\frac{(V_R - V)}{\lambda} \right) - 1 \right) \quad (8)$$

where λ is a material constant, V is the current specific volume, V_R is a reference specific volume and ℓ_0 is a measure of the granule strength. Affine deformation only changes the specific volume: the reference specific volume V_R is unchanged. Non-affine deformation changes both the reference and the actual specific volumes. It follows that, if $V_R \approx V$, there has been little or no affine deformation, suggesting that there has been very little squashing or crushing at the particle contacts. It follows that $V_R - V$ gives an indication of the hydrostatic pressure to which the material has been subjected.

For each increment, V and V_R are updated using

$$V = V(1 + \dot{e}) \quad (9)$$

and

$$V_R = V_R(1 + \dot{e}^R) \quad (10)$$

The evolution of v_i and v_r are governed by

$$v_i = -c_2 \left(\frac{V_R - V_D}{V_D} \right) \quad (11)$$

$$v_r = c_3 \left(\frac{V_L - V_R}{V_D} \right) \quad (12)$$

where c_2 and c_3 are assumed to be material constants and V_D and V_L are the densest and loosest specific volumes that the assembly can achieve at low pressure.

Clearly, given sufficiently high levels of compressive stress, one would expect that densification could occur (given that v_i is negative) by $\dot{\alpha}$ being positive. In the mathematical development that follows, these self-cancelling shear strains, because they cancel out macroscopically, are assumed to induce no work through $s_{ij} \dot{d}_{ij}^R$, purely via $\sigma \dot{e}$.

The production of flow rules and yield functions from the dilatancy rules and dissipation functions can be achieved by a number of methods surveyed elsewhere (Chandler & Sands, 2010). Here, we use the method of envelopes (Jeffrey, 2004) as in Chandler (1985).

Using the shorthand notation

$$\tilde{s}_{ij} \equiv s_{ij} + 2v_r (d_{ij}^R - d_{ij}^{\text{ref}}) \sigma \quad (13)$$

we set up an energy balance of the form

$$\phi = \tilde{s}_{ij} \dot{d}_{ij}^R + \sigma v_i (\dot{d}_{mn}^R \dot{d}_{mn}^R + \dot{\alpha}^2)^{1/2} + \sigma \dot{e}^D - \dot{D} = 0 \quad (14)$$

Then, following the procedure laid down in the theory of envelopes (Jeffrey, 2004) we obtain

$$\frac{\partial \phi}{\partial \dot{d}_{ij}^R} = \tilde{s}_{ij} + \sigma v_i \frac{\dot{d}_{ij}^R}{(\dot{d}_{mn}^R \dot{d}_{mn}^R + \dot{\alpha}^2)^{1/2}} - (\mu^2 \sigma^2) \frac{\dot{d}_{ij}^R}{\dot{D}} = 0 \quad (15)$$

$$\frac{\partial \phi}{\partial \dot{\alpha}} = \sigma v_i \frac{\dot{\alpha}}{(\dot{d}_{mn}^R \dot{d}_{mn}^R + \dot{\alpha}^2)^{1/2}} - \frac{k^2 \dot{\alpha}}{\dot{D}} = 0 \quad (16)$$

and

$$\frac{\partial \phi}{\partial \dot{e}^D} = \sigma - \frac{\ell^2 \dot{e}^D}{\dot{D}} = 0 \quad (17)$$

The flow rules are obtained by rearranging equations (15) to (17), and the yield function by eliminating the 'strain rates' from equation (14). The process depends on whether or not $\dot{\alpha} = 0$.

When $\dot{\alpha} \neq 0$

The deviatoric flow rule can be found for the case where $\dot{\alpha} \neq 0$ by first eliminating $(\dot{d}_{mn}^R \dot{d}_{mn}^R + \dot{\alpha}^2)^{1/2}$ from equation (15) using equation (16) to give

$$\dot{d}_{ij}^R = \frac{\tilde{s}_{ij}}{(\mu^2 \sigma^2 - k^2)} \dot{D} \quad (18)$$

while the yield surface can be obtained by eliminating $\dot{d}_{ij}^R$, $\dot{\alpha}$ and $\dot{e}^D$ from equation (14)

$$\psi = \left(\frac{\tilde{s}_{ij} \tilde{s}_{ij}}{(\mu^2 \sigma^2 - k^2)} + \frac{\sigma^2 v_i^2}{k^2} + \frac{\sigma^2}{\ell^2} \right)^{1/2} - 1 = 0 \quad (19)$$

as shown by the chain line in Fig. 1 for the parameter values given in Table 1. At yield, $\dot{\alpha}$ can be found by rearranging equation (16) to give

$$\dot{\alpha} = \dot{D} \left(\frac{\sigma^4 v_i^2 \mu^2 + \sigma^2 k^4 / \ell^2 - k^4}{k^4 (\mu^2 \sigma^2 - k^2)} \right)^{1/2} \quad (20)$$

Fig. 1. Sections in the $(s_{ij}s_{ij})^{1/2}/p^*$ versus $-\sigma/p^*$ plane through two yield surfaces: a cone (solid line) at low pressure and a cap (chain line) at higher pressure (see Table 1 for parameter values; $v_r=0$)

Note that $\dot{\alpha}$ loses its dependence on μ when there are no macroscopic shear strain rates.

When $\dot{\alpha}=0$.

The dissipation function when $\dot{\alpha}=0$ is

$$\dot{D} = [\mu^2 \sigma^2 \dot{d}_{mn}^R \dot{d}_{mn}^R + \ell^2 (\dot{e}^D)^2]^{1/2}$$

and the energy balance is

$$\phi = \tilde{s}_{ij} \dot{d}_{ij}^R + \sigma v_i (\dot{d}_{mn}^R \dot{d}_{mn}^R)^{1/2} + \sigma \dot{e}^D - \dot{D} = 0 \quad (21)$$

Following the standard procedure

$$\frac{\partial \phi}{\partial \dot{d}_{ij}^R} = \tilde{s}_{ij} + \sigma v_i \frac{\dot{d}_{ij}^R}{(\dot{d}_{mn}^R \dot{d}_{mn}^R)^{1/2}} - \frac{\mu^2 \sigma^2 \dot{d}_{ij}^R}{\dot{D}} = 0 \quad (22)$$

$$\frac{\partial \phi}{\partial \dot{e}^D} = \sigma - \frac{\ell^2 \dot{e}^D}{\dot{D}} = 0 \quad (23)$$

Table 1. Model parameter values for Figs 1 to 4; these figures relate to a particular material state where d^g has the values of principal strains shown in the table

Parameter	Value
μ	1.2
v_i	-0.25
v_r	0 (Figs 1–3)
	0.5 (Fig. 4)
ℓ/k	5
ℓ	2.5
d_{11}^g	1
d_{22}^g	-0.5
d_{33}^g	-0.5

equation (22) can then be rearranged to give

$$\dot{D} \tilde{s}_{ij} = \left(\mu^2 \sigma^2 - \frac{\sigma v_i \dot{D}}{(\dot{d}_{mn}^R \dot{d}_{mn}^R)^{1/2}} \right) \dot{d}_{ij}^R \quad (24)$$

Doubly contracting and square rooting both sides and then rearranging gives

$$(\dot{d}_{ij}^R \dot{d}_{ij}^R)^{1/2} = \dot{D} \frac{[(\tilde{s}_{ij} \tilde{s}_{ij})^{1/2} + \sigma v_i]}{\mu^2 \sigma^2} \quad (25)$$

Substituting this into equation (22) gives

$$\dot{d}_{ij}^R = \dot{D} \tilde{s}_{ij} \frac{[(\tilde{s}_{ij} \tilde{s}_{ij})^{1/2} + \sigma v_i]}{\mu^2 \sigma^2 (\tilde{s}_{ij} \tilde{s}_{ij})^{1/2}} \quad (26)$$

As before,

$$\dot{e}^D = \sigma \ell^2 / \dot{D} \quad (27)$$

Substituting for $\dot{d}_{ij}^R$ and $\dot{e}^D$ in the energy balance gives

$$\begin{aligned} & \frac{\tilde{s}_{ij} \tilde{s}_{ij} [(\tilde{s}_{ij} \tilde{s}_{ij})^{1/2} + \sigma v_i]}{\mu^2 \sigma^2 (\tilde{s}_{ij} \tilde{s}_{ij})^{1/2}} \dot{D} + \\ & \sigma v_i \frac{[(\tilde{s}_{ij} \tilde{s}_{ij})^{1/2} + \sigma v_i]}{\mu^2 \sigma^2} \dot{D} + \frac{\sigma^2}{\ell^2} \dot{D} - \dot{D} = 0 \end{aligned} \quad (28)$$

This can be rearranged to give the yield surface when $\dot{\alpha}=0$

$$\frac{[(\tilde{s}_{ij} \tilde{s}_{ij})^{1/2} + \sigma v_i]^2}{\mu^2 \sigma^2} + \frac{\sigma^2}{\ell^2} - 1 = 0 \quad (29)$$

which is shown by the solid line in Fig. 1.

DISCUSSION

Both these yield functions (when $\dot{\alpha}=0$ and $\dot{\alpha} \neq 0$) are plotted in Fig. 1 for the case where $v_r=0$, showing the smooth transition from the ‘cone’ to the ‘cap’ at the value of the mean stress, σ^* , the only real negative root of the right-hand side of equation (20) with $\dot{\alpha}=0$. At higher compressive mean stresses than this, the chain yield surface operates and at lower compressive mean stresses the solid yield surface operates.

In the composite yield surface, apart from at the origin, there are no vertices and there is continuity of the first derivative (though not of the second derivative). It follows that these two expressions form a two-part, continuous yield surface.

The model is fully three-dimensional and the yield surface in principal stress space, decorated with flow vectors, is shown in Fig. 2: it has a circular cross-section when cut by the constant pressure plane. Figures 3 and 4 (which also show the flow vectors) are sections in the plane of $(s_{ij}s_{ij})^{1/2}/p^*$ versus $-\sigma/p^*$ where

$$\frac{1}{p^*} \equiv \left(\frac{1}{\ell^2} + \frac{v_i^2}{k^2} \right)^{1/2} \quad (30)$$

If $v_r=0$, the hydrostatic axis is an axis of symmetry for the yield surface, as is clear in Fig. 3. When $v_r \neq 0$, the yield surface will rotate and distort (as shown in Fig. 4), but the section through the yield surface when cut by the constant pressure plane will remain circular. When $v_r \neq 0$ this choice of section in the plane $(s_{ij}s_{ij})^{1/2}/p^*$ requires some further explanation. Recall that

Fig. 2. Yield surface in dimensionless principal stress space decorated with flow vectors (see Table 1 for parameter values; $v_r = 0$)

$$\tilde{s}_{ij} \equiv s_{ij} + 2v_r(d_{ij} - d_{ij}^{\text{ref}})\sigma \quad (31)$$

An appropriate section to take in stress space is one in which

$$s_{ij} = \eta(d_{ij} - d_{ij}^{\text{ref}}) \quad (32)$$

where η is any positive number. A section through the yield surface can then be written using the shorthand $d_{ij}^g \equiv d_{ij} - d_{ij}^{\text{ref}}$ as

$$0 = \left(\frac{[(s_{ij}s_{ij})^{1/2} + 2v_r\sigma(d_{ij}^g d_{ij}^g)^{1/2}]^2}{(\mu^2\sigma^2 - k^2)} + \frac{\sigma^2 v_i^2}{k^2} + \frac{\sigma^2}{\ell^2} \right)^{1/2} - 1 \quad (33)$$

which makes use of the relation

$$s_{ij}d_{ij}^g \leq (s_{ij}s_{ij})^{1/2}(d_{ij}^g d_{ij}^g)^{1/2} \quad (34)$$

which is an equality when equation (32) is obeyed. Different dissipation functions would produce different shaped cones, as explained elsewhere (Chandler & Sands, 2009; Sands & Chandler, 2010). The values of the parameters are restricted.

Fig. 3. Section through the composite yield surface with flow vectors, $\frac{1}{p^*} = \left(\frac{1}{\ell^2} + \frac{v_i^2}{k^2} \right)^{1/2}$ (see Table 1 for parameter values; $v_r = 0$)

Fig. 4. Section through the composite yield surface with flow vectors, $\frac{1}{p^*} = \left(\frac{1}{\ell^2} + \frac{v_i^2}{k^2} \right)^{1/2}$ (see Table 1 for parameter values; $v_r = 0.5$)

Equation (16) shows that for non-zero α , v_i must be negative. It is also clear from the energy balance (equation (14)) that $v_i + \mu > 0$. If this is not the case, the granular packing can collapse under any arbitrarily small positive pressure. Such collapses occur as granules first settle in a container. This model only simulates the compaction that occurs after this initial collapse.

The values of the specific volumes V , V_L and V_D can be established experimentally from standard tests. The rest of the model parameters can be determined by running a number of simulations and comparing them with experimental results.

- ℓ_0 and λ are chosen to give a good fit to the isotropic compression line determined from an experiment on sand vibrated under low pressure to its maximum initial density. At the zero pressure limit of this test, $V = V_R$.
- ℓ/k and c_2 are chosen to give a good fit to similar tests carried out on a range of looser samples.

Fig. 5. Vertical (K_0) compression tests by Northcutt (2010) (solid lines) carried out on Fraser River sand at various initial packing densities. The broken lines show simulations using the model parameter values in Table 2. Note that the initial slope increases with initial void ratio

Table 2. Parameters for Figs 5 to 8. The material in Figs 6–8 was pre-compacted to 100 kPa but prior to that had $V = 1.85$, $V_R = 1.852$ (a moderately loose packing). Fig. 8 uses values of V and V_R for moderately loose sand.

Parameter	Value
c_1	8.0
c_2	1.0
c_3	35
μ	0.636
ℓ/k	0.18
ℓ_0	1.4 kPa
V_L	1.962
V_D	1.62
V (initial)	1.666, 1.751, 1.85, 1.954
V_R (initial)	1.668, 1.753, 1.852, 1.956
λ	0.004

- c_1 , c_3 and μ are determined from low-pressure shear tests (e.g. triaxial compression tests or hollow cylinder torsion tests): c_1 determines the magnitude of the shear strain needed to reach the critical state; c_3 determines the density at the critical state; μ is the value of the shear stress invariant at the critical state.

SIMULATIONS

Figure 5 shows the results (solid lines) of experiments in vertical (K_0) compression by Northcutt (2010) on initially very loose, moderately loose, moderately dense and very dense Fraser River sand. Note that the slopes at low pressure increase with initial void ratio, reflecting the greater opportunity to densify by rearrangement. Simulations of those experiments, produced using the model presented here with the parameter values given in Table 2, are superimposed on the experimental results using broken lines. The agreement is good and shows that the model is capable of capturing the influence of initial density.

Figures 6 to 8 show the results (redrawn) of cyclic shear experiments carried out by Sriskandakumar (2004) on nominally identical samples of moderately loose Fraser River sand. Each sample of sand was vertically consolidated to 100 kPa ($D_r = 40\%$) and then cyclically sheared, with no lateral strain and a constant vertical stress of 100 kPa, using different maximum shear strains ($\pm 8\%$, $\pm 4\%$ and $\pm 2\%$).

Fig. 6. Results of an experiment by Sriskandakumar (2004) (solid lines) on a sample of moderately loose Fraser River sand ($D_r = 40\%$) consolidated vertically to 100 kPa and then sheared cyclically to $\pm 8\%$ shear strain amplitude. The broken lines show simulations using the model parameter values in Table 2

Fig. 7. Results of an experiment by Sriskandakumar (2004) (solid lines) on a sample of moderately loose Fraser River sand ($D_r = 40\%$) consolidated vertically to 100 kPa and then sheared cyclically to $\pm 4\%$ shear strain amplitude. The broken lines show simulations using the model parameter values in Table 2

Simulations of those experiments, run using the model presented here with parameter values shown in Table 2, are superimposed on the experimental results using broken lines. A least-squares (Sands *et al.*, 2011) optimisation technique was used to determine the unspecified stress and strain increment. As one would expect, minor discrepancies between the experiments and the simulations build up with each cycle, but the overall agreement is good, demonstrating the suitability of the dilation rule.

CONCLUDING REMARKS

This letter introduces the concept, which is still being explored, of self-cancelling shear strains. We postulate that shear strains present at the microstructural level might be sufficient to account for compaction under pressure alone while cancelling each other out to the extent that there is negligible macroscopic shear strain. At this stage in the development of this concept, it is anticipated that it could be most usefully applied to soils experiencing low to moderate pressures.

Fig. 8. Results of an experiment by Sriskandakumar (2004) (solid lines) on a sample of moderately loose Fraser River sand ($D_r = 40\%$) consolidated vertically to 100 kPa and then sheared cyclically to $\pm 2\%$ shear strain amplitude. Simulations, using the properties given in Table 2, are shown with broken lines

The concept has been incorporated into a material model and successfully used to simulate compaction and cyclic shear tests carried out by others, achieving encouraging agreement with the experimental results. Work on more detailed comparison with experimental data is ongoing.

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