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A simple micro-inspired model for granular materials made of hollow crushable particles.

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Abstract. This paper presents a new macroscopic constitutive model for granular materials constituted by hollow, crushable particles. Inspired by micromechanical data, the model extends the Sinfonietta-Classica elastoplastic model to incorporate particle breakage and the resulting compaction. The behaviour of the material is characterised by three distinct regimes: initial rigidity, high compressibility due to particle crushing, and subsequent post-breakage stiffening. The model relies on a relationship between volumetric strain and the fraction of broken particles, captured by a microscopically informed smoothed transition function. A numerical simulation under oedometric conditions is carried out to validate the model, to evaluate its ability to reproduce discrete element method (DEM) results. The proposed approach allows for the derivation of new parameters using DEM simulations, while classical parameters can be determined through standard tests on the fully crushed material. Future work aims to generalize the model to account for finite deformation, diverse loading paths, and compaction bands formation.

1 Introduction

Many products in the food industry, such as macaroni noodles or breakfast cereals, consist of granular materials made of hollow crushable particles. Similarly, in the energy sector, coal power plants produce hollow glass beads known as cenospheres, which find applications in the construction industry, including thermal insulation, lightweight composite materials, and concrete. When stored in large silos, these granular materials experience stress levels that can lead to particle breakage, significantly influencing their mechanical behaviour. While continuum approaches to model granular material breakage have been widely developed over the past few decades [1–4], to our knowledge, the specific case of hollow particles has yet to be addressed from a continuum mechanics perspective.

In this work, we propose an extension to the existing plasticity model Sinfonietta-Classica, originally formulated by Roberto Nova [5], to incorporate the breakage of hollow particles as a degradation mechanism. In such a granular medium, we consider that the primary consequence of breakage is kinematic: when a particle fractures, its internal void space becomes available for further deformation. This assumption leads to a distinction between two porosity components: the porosity available and non-available for deformation. Inspired by damage mechanics [6], we assume that the available porosity increases with grain breakage and follows an evolution law expressed as a function of deformation. This evolution law is derived from micro-scale geometrical considerations and supported by Discrete Element Method (DEM) simulations. We further reformulate the hardening law of the model as a porosity-dependent expression that depends solely on the open porosity available for deformation. A numerical simulation under oedometric conditions is conducted using an engineered granular material composed of brittle baked clay tubes [7], also analyzed through DEM. The results demonstrate that the proposed model effectively captures the key features of the material mechanical response, providing a framework for improved predictive modelling of granular materials composed of hollow crushable particles.

2 A micro-mechanical inspiration

The model material considered in this study is a granular assembly of hollow tubes made of baked clay. The behaviour of this material have been studied experimentally, under oedometric conditions, in previous works by Stasiak *et al.* [7], and the main deductions have been underpinned by numerical experiments carried out with the discrete element method (DEM). It has been shown that the main features of the behaviour of the material is a strong non-linearity caracterised by three different regimes depending on the stress level. For lower stress levels the first phase shows a rather classical behaviour of a granular material made of rigid particles with elasto-plastic interactions. For intermediate stress levels, the material shows a large compressibility, say a sudden increase in deformation associated to small stress variations. This behaviour is attributed to the crushing of the particles which induces a collapse of the assembly. Once all the particles have been broken, the material retrieves a larger stiffness and shows once again

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a standard hardening plastic behaviour of a granular material. The DEM simulations captured the evolution of the particle breakage during the loading and suggested a link between the volumetric deformation ε_v and the fraction b of broken particles such that $b = b(\varepsilon_v)$, which we propose to approach by the following smoothed transition function:

$$b(\varepsilon_v) = \left\langle -\frac{\varepsilon_v}{\varepsilon_v^k} - \frac{\omega \ln\left(1+\exp\left(-\frac{\varepsilon_v+\varepsilon_v^k}{\omega}\right)\right)}{\varepsilon_v^k} \right\rangle_+ \qquad (1)$$

where $\langle\cdot\rangle_+$ denotes the postitive part operator. The quantity ε_v^k is the characteristic strain for which the functions observes a break in slope (knee) that corresponds to the strain for which almost all the tubes are broken. The non-dimensional quantity ω controls the hardness of the knee. This expression is illustrated in Figure 1.

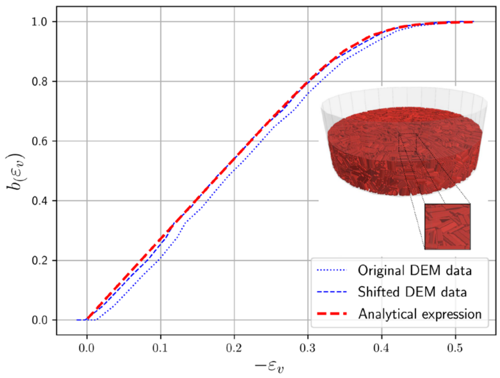

Figure 1. Model for the evolution of the fraction of broken particle with respect to the volumetric strain for $\varepsilon_v^k = 0.37$ and $\omega = 0.035$ (dashed red line). DEM data (dotted blue line) are collected from [7] (see Figure 18 herein). The DEM data used for calibration (dashed blue line) has been shifted in order to force the intersection with the point (0,0). The DEM sample representation comes from [7], figure 17

We take inspiration from this available micromechanical data to build a macroscopic model. We consider, in addition, that the pore space that is circumscribed inside a tube is not accessible unless the tube is broken. This assumption leads to introduce ϕ^b as the porosity (say the volume fraction of the pore space) that is made available for deformation after breakage, see Figure 2. In terms of kinematics, we consider that this additional porosity modifies the reference available porosity ϕ_0^a. Considering that the individual tubes that composes the granular assembly, and the matrix they composes them, are not compressible, we express the so-called grain incompressibility condition as a restriction between the volumetric strain ε_v and the porosity variations:

$$\varepsilon_v = \phi - \left(\phi_0^a + \phi^b\right) \qquad (2)$$

where ϕ is the current porosity available for deformation. The term ϕ^b is then micro-informed stating that the additional pore space available for deformation after breakage is proportional to the fraction of broken tubes: $\phi^b = \phi_\infty^b b(\varepsilon_v)$ where we introduce ϕ_∞^b as the maximum breakage induced porosity, which is defined as the initial volume fraction of the pore space contained inside the particles, with respect to the sample total volume. The interpretation of each term of equation (2) in terms of reversible and non-reversible contributions will be discussed further in section 3. The assumption proposed here is reasonable if the geometry of the particles does not show excessive variability. It is worth to notice that in that case and starting from DEM samples, ϕ_∞^b can be constructed from the sole knowledge of the initial shape of the particles, their number, and the size of the whole sample. This formulation is now an interesting starting point to build a micro-informed macroscopic constitutive model.

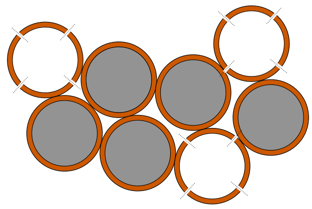

Figure 2. Schematic representation of the porosity made available after grain breakage. The grey filled circles are intact tubes and the white filled ones are broken: their inner pore space is released and then available for further deformations

3 Macroscopic elastoplastic model

In order to build a macroscopic model, we propose to extend an existing elasto-plastic model and to incorporate the particle breakage released porosity discussed in the previous section, as an additional plastic evolution source. The model we proposed to extend is the non-associated plasticity model Sinfonietta-Classica proposed by Roberto Nova to capture mechanical behaviour of sandy soils, and which bridges the original Cam-Clay model and the Matsuoka Nakai failure criterion. In this work we specify only the part of the model that we propose to extend, and the reader may find a complete presentation of the original model in [5]. The index notation is used for tensors. First, we assume that the elastic behaviour of the material is non-linear and governed by a Cam-Clay like equation, see Borja *et al.* [8]. The strain tensor is split into an elastic tensor ε^e and a plastic one ε^p such that $\varepsilon_{\alpha\beta} = \varepsilon^e_{\alpha\beta} + \varepsilon^p_{\alpha\beta}$. The variation of the stress tensor $\boldsymbol{\sigma}$ reads then as:

$$\dot{\sigma}_{\alpha\beta} = 2\mu\left(\dot{\epsilon}_{\alpha\beta} - \dot{\epsilon}^p_{\alpha\beta}\right) + \lambda\left(\dot{\varepsilon}_v - \dot{\varepsilon}^p_v\right)\delta_{\alpha\beta} \qquad (3)$$

with $\varepsilon_v = \varepsilon_{\gamma\gamma}$, $\varepsilon_v^p = \varepsilon^p_{\gamma\gamma}$, $\epsilon_{\alpha\beta} = \varepsilon_{\alpha\beta} - \varepsilon_v\delta_{\alpha\beta}/3$ and $\epsilon^p_{\alpha\beta} = \varepsilon^p_{\alpha\beta} - \varepsilon^p_v\delta_{\alpha\beta}/3$, $\delta_{\alpha\beta}$ being the Kronecker symbol. Moreover, in this constitutive equation, μ and λ denote the shear modulus and the first Lamé coefficient respectively:

$$\mu = \frac{3K(1-2\nu)}{2(1+\nu)}, \quad \lambda = \frac{3K\nu}{(1+\nu)} \qquad (4)$$

ν being the Poisson ratio of the material, and K the mean stress dependent bulk modulus:

$$K = -\frac{1+e_0}{3\kappa}\sigma_{\gamma\gamma}, \tag{5}$$

with κ the logarithmic volumetric compliance of the material, and e_0 the reference void ratio, defined as the ratio between the pore volume fraction and the solid volume fraction, which can be calculated as a function of the initial porosity: $e_0 = \phi_0/(1-\phi_0)$, where ϕ_0 is the initial porosity, accounting for both available and non-available pore space. As in any classical elastoplastic model, the yielding of the material is decided by means of a yield function: If f and its differential $\dot{f}$ equal 0, then the material yields. In the Sinfonietta-Classica model, the yield function is defined as a function of the stress state $\boldsymbol{\sigma}$ and the preconsolidation pressure p_c which plays the role of a hardening force which evolves following a hardening law given in terms of the plastic strain variation $\dot{\varepsilon}^p$:

$$\frac{\dot{p}_c}{p_c} = \frac{1}{\beta_p}\left(-\dot{\varepsilon}_v^p + \varkappa\dot{\epsilon}_c^p\right) \tag{6}$$

where β_p is a hardening compliance and $\varkappa$ a parameter that controls the influence of plastic distorsion on the hardening. The term $\dot{\epsilon}_c^p$ represents the variation of the cumulated plastic strain such that $\dot{\epsilon}_c^p = \sqrt{\dot{\epsilon}_{\alpha\beta}^p\dot{\epsilon}_{\alpha\beta}^p}$. As the model is non-associated, the evolution of the plastic strain tensor is given by means of a plastic potential g such that $\dot{\varepsilon}^p = \gamma g_{,\sigma}$ where γ denotes the so called *plastic multiplier* and $g_{,\sigma}$ the gradient of g in the stress tensor space. Detailed formulation of the yield function and plastic potential are given in appendix 5.

In porous material without any degradations, if the matrix is not compressible, it is possible to identify the volumetric plastic strain variation with the irreversible part of the variation of the open porosity that we denote $\dot{\phi}_{in}$. As a consequence it is possible to refomulate the hardening law as:

$$\frac{\dot{p}_c}{p_c} = \frac{1}{\beta_p}\left(-\dot{\phi}^{in} + \varkappa\dot{\epsilon}_c^p\right) \tag{7}$$

This formulation constitutes a simple change in point of view that allows to enrich the hardening law by any source of non-reversible porosity. In our case, from the micromechanical arguments we developped in section 2, we consider that the particle breakage provides a non-reversible increase in the open porosity that we denotes ϕ^b so that we consider $\dot{\phi}^{in} = \dot{\phi}^b + \dot{\varepsilon}_v^p$ and the hardening law becomes:

$$\frac{\dot{p}_c}{p_c} = \frac{1}{\beta_p}\left(-\dot{\varepsilon}_v^p - \dot{\phi}^b + \varkappa\dot{\epsilon}_c^p\right) \tag{8}$$

The model being formulated, it is possible to incorporate microscopic information obtained from DEM simulations by considering a relationship between ϕ^b and the strain as mentioned is section 2. Moreover, as the granular materials often exhibits low elastic strain with respect to the plastic strain, we propose to express the relationship in terms of *plastic* volumetric strain ε_v^p, so that:

$$\phi^b = \phi_\infty^b b\left(\varepsilon_v^p\right) \tag{9}$$

which completes the model formulation.

Table 1. Material parameters used for the oedometric simulations

κ	ν	e_0	$p_{c0}\,[kPa]$	β_p
0.0275	0.2	2.44	60	0.038
ϕ_∞^b	ε_v^k	ω	$\varphi\,[deg]$	β
0.29	0.37	0.035	31.5	3

4 Numerical simulations

In order to illustrate the model abilities, a numerical simulation is carried out with the aim of reproducing the numerical results obtained in oedometric conditions using the DEM by Stasiak *et al.* [7]. The material parameters used in this study are reported in Table 1. The model should reproduce the behaviour of the material once all the particles are broken, which gives a guide to determine the material parameters: most of the materials parameters that concern the classical part of the model (say κ, ν, φ, β, β_p), should be calibrated from experimental or DEM tests carried out over the material that results from the crushing of all of the particles. The parameters ϕ_∞^b, ε_v^k and ω derive from numerical data from Stasiak *et al* [7]. The calculation is achieved using the finite element software FEniCS [9] for which an elasto-plasticity library have been developped in Laboratoire 3SR. The domain used for this calculation is a rectangle of $0.13\,m \times 0.35\,m$, and its finite element mesh made of 210 second order triangular elements. To stay representative of oedometric conditions, the vertical displacement of the bottom edge is set to zero, as for the horizontal displacement of the lateral edges. Plane strain hypothesis holds, in order to capture the 3D nature of the problem. In terms of loading, the compression of the sample is achieved by means of an incremental downward vertical displacement of intensity u_d with an intensity up to $17.5\,mm$. Additionally, two unloading and loading cycles are considered, with vertical displacement amplitude of $3.15\,mm$. A schematic representation of the mesh and boundary conditions is given in Figure 3. The results of

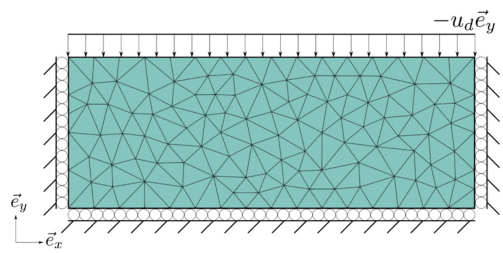

Figure 3. Schematic representation of the mesh and boundary conditions considered for the finite element calculations

the simulations are reported in Figure 4. From this figure, we first observe that the model is able to reproduce, stress fluctuation asides, the three different behaviour regimes exhibited by the DEM material: initial rigidity (for stress levels bellow $20\,kPa$ and $200\,kPa$), high compressibility due to particle crushing (for stress levels between $200\,kPa$ and $1500\,kPa$), and subsequent post-breakage stiffening (for stress levels above $1500\,kPa$). Moreover, we observe that the response of the model is close to that of the DEM material, showing the ability of the model to reproduce quantitatively the response of the material. The transition between the high compressibility regime and the post-breakage stiffening is observed for deformation between 0.35 and 0.45, which coincides with the knee observed in the $b(\varepsilon_v)$ relationship, see Figure 1. Finally, the model is also able to capture qualitatively and quantitatively the response of the material during unloading scenarii, initiated in the second and third regimes aforementioned.

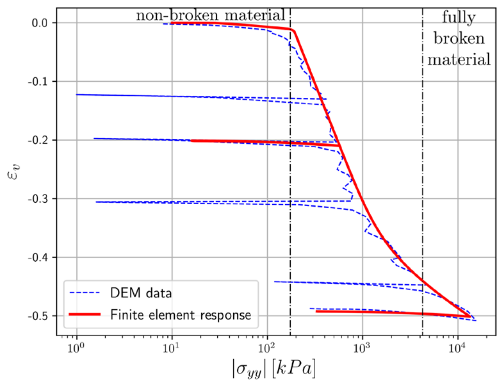

Figure 4. Response of the model to oedometric loading (red line), compared with DEM data collected from Figure 17 in [7] (dashed blue line).

5 Conclusions

In this work we proposed a macroscopic constitutive model for a granular material made of crushable hollow particles which is based on a existing model extended by considering geometrical arguments derived from breakage kinematics at the microscopic scale. The model is compared to existing results in oedometric conditions and it has been shown that it is able to represent well the behaviour of the material. One key advantage of this new model is that the new parameters are micro informed and can be derived from DEM simulations whilst the other parameters can be calibrated with respect to classical tests (oedometric and triaxial tests) carried out over the material resulting from the complete crushing of the particles. Further works will be devoted to the generalization of the model in order to (i) consider finite deformation (ii) provide a thermodynamically consistent formulation (iii) account for diverse loading paths (iv) reproduce possible compaction bands formation due to grain crushing, implying the use of an enriched continuum description.

Appendix. Yield function and plastic potential

In the model Sinfonietta-Classica, the yield function f and plastic potential g are given by:

$$f(\boldsymbol{\sigma}, p_c) = 3\beta(\gamma-3)\ln\frac{3p_c}{\sigma_{\gamma\gamma}} + \frac{9}{4}(\gamma-1)J_{2\xi} + \gamma J_{3\xi}, \quad (10a)$$

$$g\left(\boldsymbol{\sigma}, p_g\right) = 9(\gamma-3)\ln\frac{3p_g}{\sigma_{\gamma\gamma}} + \frac{9}{4}(\gamma-1)J_{2\xi} + \gamma J_{3\xi}, \quad (10b)$$

where β is a material parameter characterising the non-associativity (for $\beta = 3$ the model is associated) and p_g is a parameter being of no interest as only the gradient of g appears in the calculations. The parameter γ is related to the characteristic state of the material:

$$\gamma = \frac{9-M^2}{3-M^2+2M^3/9}, \quad \text{with} \quad M = \frac{6\sin\varphi}{3-\sin\varphi} \quad (11)$$

φ being the friction angle at characteristic state, defined as set of stress and hardening states for which $\dot{\varepsilon}_v^p = 0$. The quantities $J_{2\xi}$ and $J_{3\xi}$ refers to the stress tensor invariants. Denoting $\boldsymbol{s}$ the deviatoric stress tensor such that: $s_{\alpha\beta} = \sigma_{\alpha\beta} - \frac{\sigma_{\gamma\gamma}}{3}\delta_{\alpha\beta}$ and then the stress ratio tensor ξ such that: $\xi_{\alpha\beta} = -3s_{\alpha\beta}/\sigma_{\gamma\gamma}$, $J_{2\xi}$ and $J_{3\xi}$ reads as:

$$J_{2\xi} = \xi_{\alpha\beta}\xi_{\alpha\beta} \quad \text{and} \quad J_{3\xi} = \xi_{\alpha\beta}\xi_{\beta\gamma}\xi_{\gamma\alpha} \quad (12)$$

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