A multiscale approach for cohesive and unsaturated soils as a constitutive model designed for FLAC3D

Marie Miot¹, Guillaume Veylon¹, Antoine Wautier¹, Sacha Emam², François Nicot³ & Pierre Philippe¹
¹ Irstea, Aix Marseille Univ, RECOVER, 3275 Rte Cézanne, CS 40061, 13182 Aix-en-Provence Cedex 5, France
² Itasca Consultants, S.A.S., 64 Chemin des Mouilles, 69134 Ecully, France
³ Université Grenoble Alpes, Irstea, UR ETGR, 2 rue de la Papeterie-BP 76, St-Martin-d’Hères

1 INTRODUCTION

Mechanical modelling of granular material at large scale, such as in the case of hydraulic structure, gives rise to some issues inherent to the microstructure effects, which are generally not accounted for in classical constitutive laws implemented in continuous models. Coupling Finite Element Method, at the scale of the structure, and Discrete Element Method (DEM), at the scale of a Representative Elementary Volume (REV), can account for these effects, but is computation time demanding. In this respect, multiscale models, in which the constitutive behavior of a material is deduced from statistical homogenization, provides interesting perspectives. Such models can indeed account for microstructure effects at a lower computation cost.

The H-model, developed in (Nicot & Darve 2011, Veylon 2017, Xiong 2017) is an example of such models. In the 3D-H-model, the mesostructure is a bi-hexagon constituted of ten grains. The hypothesis made on the geometry and symmetry of the bi-hexagon make it possible to link analytically the forces to the displacements at the mesoscale, and the stresses to the strains at the macroscale thanks to a directional homogenization process.

So far, this model has been validated against experimental tests only for dry cohesionless granular materials. We present here an extension under development of the 3D-H-model, which includes the effects of both solid cohesion, and water content to model unsaturated soils and possibly internal erosion processes. In this paper, the classical 3D H-model is first reviewed. Then, the different extensions of the model are presented, and implementation details are given. Finally, a validation process is proposed, by comparison against experimental or numerical results provided by other constitutive relations.

2 REVIEW OF THE H-MICRODIRECTIONAL MODEL

The 3D-H-model is a multiscale model that defines in an implicit way the constitutive law between strains and stresses for dry cohesionless soils. This model introduces a mesoscale constituted by a mesostructure of ten grains in 3D (Fig. 1), which is supposed to capture important microscale mechanisms at stake in granular materials.

The ten grains of the mesostructure have the same radius, and their centers form two hexagons in two orthogonal planes. Considering all the symmetries in the bi-hexagon, in terms of geometry and external forces, the geometry of the bi-hexagon can be entirely described by the opening angles $\alpha_1$ and $\alpha_2$ of the two hexagons, and the distance $d_1$, $d_2$, $d_3$ and $d_4$ between the centers of the grains in the two patterns (Fig. 1). These symmetries make it possible to express analytically the overall stress tensor as a function of the overall incremental strain tensor (Xiong 2017).
The incremental computation scheme of the model is presented in Figure 2. First, the incremental strain tensor $\delta \vec{\varepsilon}$ is recovered in FLAC3D (Itasca 2017) for each mesh cell. The incremental lengths of each bi-hexagon are deduced by projecting the global strain along the axial direction:

$$\delta \vec{L} = \begin{bmatrix} \delta l_1 \\ \delta l_2 \\ \delta l_3 \end{bmatrix} = \vec{P} \delta \vec{\varepsilon} \vec{P}^{-1} \vec{L}$$

(1)

where $\vec{P}$ is the rotation matrix from global ($\vec{x}, \vec{y}, \vec{z}$) to local frame ($\vec{n}, \vec{t}, \vec{w}$), and $\vec{L}$ describes the current geometry of the bi-hexagon.

The geometrical compatibility relations in the hexagons link the lengths of the branch vectors $d_i$ and the opening angles $\alpha_i$ of the cell at the microscale with the lengths of the hexagons $l_i$ at the mesoscale, as follows:

$$\begin{aligned}
l_1 &= d_2 + 2d_1 \cos \alpha_1 = d_4 + 2d_3 \cos \alpha_2 \\
l_2 &= 2d_1 \sin \alpha_1 \\
l_3 &= 2d_3 \sin \alpha_2
\end{aligned}$$

(2)

At the microscale, an elasto-frictional contact law operates between grains. The contact forces are related to the opening angles and the lengths of the branch vectors, in both elastic and plastic regimes:

$$\begin{aligned}
\delta N_i &= -k_n \delta d_i \\
\delta T_i &= k_i d_i \delta \alpha_j & \text{if } |T_i + \delta T_i| < (N_i + \delta N_i) \tan \phi_g \\
\delta T_i &= \pm k_n \tan \phi_g \delta d_i & \text{if } |T_i + \delta T_i| = (N_i + \delta N_i) \tan \phi_g
\end{aligned}$$

(3)

The equilibrium equations for the grains 1, 2 make it possible to link the external forces at the mesoscale to the contact forces at the microscale:

$$\begin{aligned}
F_1 &= 2(N_1 \cos \alpha_1 + T_1 \sin \alpha_1) + 2(N_3 \cos \alpha_2 + T_3 \sin \alpha_2) \\
F_2 &= N_1 \sin \alpha_1 - T_1 \cos \alpha_1 \\
N_2 &= N_1 \cos \alpha_1 + T_1 \sin \alpha_1 + G_2 \\
G_2 &= T_2
\end{aligned}$$

(4)

Finally, the incremental forces in a bi-hexagon with orientation $(\theta, \phi, \psi)$ are obtained from Equations (2)-(4).

The stresses at the mesoscale are obtained with the Love-Weber formula:

$$\sigma_{ij}^h = \frac{1}{V} \sum_{c=1}^{N_c} F_i^c l_j^c$$

(5)
Where $N_c$ is the number of contacts in the mesostructure, $F_i^c$ the $i^{th}$ component of the forces and $l_j^c$ the $j^{th}$ component of the branch vector at contact $c$.

Then, the macroscopic stress tensor in the REV is obtained by performing a statistical homogenization along all the spacial directions:

$$
\bar{\sigma} = \frac{1}{V_{tot}} \iiint \omega(\theta, \phi, \psi) \bar{p}^{-1} V \bar{\sigma}_h \bar{p} \sin \phi \, d\phi \, d\theta \, d\psi \quad V_{tot} = \iiint \omega V(\theta, \phi, \psi \sin \phi \, d\phi \, d\theta \, d\psi)
$$

with $\omega$ the distribution function of the directions.

Figure 2. Resolution scheme of the H-microdirectional model. 3D H-model (solid lines), extension to solid cohesive material (dotted lines), capillary correction (dashed lines), erosion model correction (dash-dot lines).

3 EXTENDED H-MODEL

3.1 Solid cohesion

Solid cohesion affects the mechanical behavior of a granular material but has not been implemented in the first version of the H-model presented in the previous section.

The solid cohesion may be due to the cementation of compounds present in water, or to the crystallization of salts, which tends to form solid bridges between grains (Soulié 2005). In the extended H-model, the solid cohesion is implemented at the scale of the contact between grains, using normal and tangential cohesions $c_n$ and $c_t$, in addition to the friction angle $\phi_g$ (Fig. 2).

In the initial state, solid bonds are created between the grains in contact. The contact behaves in the elastic regime while:

$$
\begin{cases}
\{ |T_i| \} = c_t + N_i \tan \phi_g \\
N_i \geq -c_n
\end{cases}
$$

Otherwise, the bond is broken, and the contact becomes purely frictional. In the computation scheme presented previously, eq. (3) is modified according to (7).
3.2 Capillary forces

In many cases real soils are neither dry nor fully saturated. This partially saturated state is not accounted for in the current H-model.

In unsaturated soils, different regimes can be distinguished:

- In pendular regime, for small degrees of saturation, water forms independent capillary bridges between grains.
- For higher degrees of saturation, capillary bridges merge and form clusters of water in a continuous gas phase, which defines the funicular regime.
- The loss of continuity in the gas phase marks the onset of the capillary regime.

In the extended H-model, the global degree of saturation will be used to determine a statistical repartition of the volume of water in the different cells.

Capillary forces are calculated as in (Miot et al. 2019) using a surface energy minimization approach with the gradient descent method implemented in the software Surface Evolver (Brakke 1992). Several abacuses are created in order to relate the capillary forces and the water regime at the mesoscale as a function of the mean opening angle $\alpha$ and the volume of water $V_w$ in the cell. Knowing these parameters, the capillary forces are determined and applied to each mesostructure as external forces, as shown in Figure 2.

3.3 Erosion modeling

Internal erosion processes are an important issue for widely graded soils in which the presence or absence of free particles affects the mechanical behavior of the soil. As free particles have a large impact on the stability of granular media (Wautier et al. 2018), their contribution should not be neglected contrary to what is implicitly assumed in the current H-model, with monodisperse grain size and no free particles. In the extended H-model, a volume $V_r$ of granular material composed of smaller particles is added into the void of the cell. While the inner volume $V$ of the cell is larger than $V_r$, the small particles do not participate to stress transmission and the behavior of the H-model remains unchanged.

But, as soon as $V < V_r$, the small particles will apply additional contact forces on the inner part of the cell. The inner contacts thus created are assumed to be non-frictional and characterized by a normal stiffness such that the inner volume of fine particles behave as a continuous material of compressibility modulus $K$. Such reasoning enables to relate the normal contact stiffness of the 10 inner contacts to the volume variation ($V_r - V$) and $K$.

The threshold volume $V_r$ is determined with the total void ratio $e$, while the intergranular void ratio $e^\theta$, as defined in (Benahmed et al. 2015) gives the initial opening angle of the cells. The stiffness coefficient $K$ can be calibrated for instance with DEM simulations. Internal erosion of the material is then modelled by removing smaller particles through a decrease in $V_r$.

4 MODEL VALIDATION

Some comparative tests will be performed using FLAC3D in order to validate the constitutive law. As the 3D H-model has already been validated in (Xiong 2017), the new tests will focus specifically on the additional validation of the extended H-model.

First, the solid cohesive model can be compared with DEM results of triaxial tests for a REV of bonded granular materials with varying tensile limit. Experimental tensile and shear tests with glass beads and paraffin bonds will also be available for comparison.

The capillary model will be validated with experimental tests found in the literature, such as the shear tests presented in (Cuomo et al. 2016).

Finally, the impact of free particles will be assessed by comparing numerical and experimental drained triaxial tests in (Aboul Hosn 2017, Nguyen 2018) and directional analysis as presented in (Wautier et al. 2018).
REFERENCES


