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▶ To cite this version:

Nuria M Pinyol. CONSTITUTIVE MODELLING OF BONDED EXPANSIVE GEOMATERIALS. W(H)YDOC~08:~3rd international workshop of young doctors in geomechanics, Nov 2008, Champs-sur-Marne, France. pp. 55-58. hal-00510414

HAL Id: hal-00510414

https://hal.science/hal-00510414

Submitted on 18 Aug 2010

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CONSTITUTIVE MODELLING OF BONDED EXPANSIVE GEOMATERIALS

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ABSTRACT. This paper presents a discussion on existing approaches to derive constitutive models for bonded geomaterials conceived as composite materials. The methodology involves the partitioning of strains, the adoption of constitutive models of constituents and the integration of component stresses into the external stress. These steps are guided by microstructural observations, but are open to alternative formulations which are part of the overall constitutive behaviour.

1. Materials involved

Soft clay rocks and hard soils clay soils are well known examples of bonded materials often found in engineering works. Their structure is the result of a particular mineralogy, a diagenetic process and a subsequent geological history, most notably, the tectonic history. A common observation is than weathering action as well stress changes lead to a material degradation which is associated with two phenomena:

- The release of the expansion potential of clay minerals
- The loss of strength and continuity of internal bonds

The bonding process generally occurs when the parent clayey soil is under stress. A consequence of this process is that any unloading may lead to bond breakage. In addition, hydration of clay stacks may reverse the initial consolidation of sediments and lead also to bond breakage. A few examples of bonded expansive materials are weathered old alluvium soil from San Juan, Puerto Rico (Zhang *et al.*, 2004), the tertiary mudrocks from the French Central Massif (Pejon and Zuquette, 2002), the Callovo-Oxfordian claystone from Eastern France (Zhang *et al.*, 2004), the Opalinus clay from Northern Switzerland (Muñoz, 2007) among many others.

ESEM photographs provide some clues on the organization of the microstructure. Porosimetry and mineral identification provide also information which could be used to build a conceptual model of the soil microstructure. A variety of additional chemical and physical test are available to investigate the micro fabric (see Zhang *et al.*, 2004). However deciding the fundamental nature of a given microstructure, within the perspective of constitutive modelling remains a highly speculative exercise. Decisions at this fundamental level will have a strong influence of the macroscopic behaviour derived form the model. This paper investigates possible relationships for bonded expansive geomaterials.

2. Some experimental observations

As a general rule, the intensity of bonding, which may be simply measured by the concentration of the bonding material, increases the stiffness and the strength of the material. In a more general sense, the yielding locus expands when bonding is present. This is usually shown by comparing the compressive behaviour of intact and remoulded specimens. Yielding means the rupture of bond connections but also a loss of the intact initial geometric arrangements of the microstructure. It is often found also than under increasing loading the material approaches the behaviour of the fully unbonded/unstructured material.

Additional laboratory observations and field evidence indicates that stress changes damage the bond and allows the release of the swelling potential. The application of repeated loading-unloading cycles enhances the bond breakage and the soil degradation. Suction cycles are also particularly effective in degrading these materials. This is shown by Wong (1998) which showed the complete loss of brittleness and strength of clay shales subjected to suction cycles.

3. Conceptual representation of microstructure and modelling

The following approaches have been reported in the literature for the development of constitutive models:

A suitable modification of a "standard" constitutive model valid for unstructured or debonded soils.
 Examples of this kind are the proposals of Gens & Nova (1993), Kavvadas & Amorosi (1998), Baudet & Stallebrass (2004).

- Integrate damage and elastoplasticity concepts into the model formulation (Chazallon and Hicher, 1995; Chiarelli *et al.*, 2003).
- Interpreting the material microstructure and building a macroscopic model from some basic simple models which are believed to represent the material constituents. Typically the bonded material is assumed to be composed by two components: grains (or clay aggregates) and bond. For instance, Chazallon and Hicher (1998) conceived the bonded material as the response "in parallel" of two elastoplastic materials, one of them capable to experiencing damage. Other examples are provided by Vaunat and Gens (2003) and Zhang et al. (2004). This is also the approach followed in this work. The clay matrix will be identified as an expansive material represented by the double structure elastoplastic model for unsaturated clays known also as Barcelona Expansive Model (BExM) (Alonso et al., 1999). The bond will be characterized by a quasi-fragile material described by Carol et al. (2001).

4. Conceptual representation of microstructure and modelling

Phenomenological models rely on the intuition of the authors, an intuition which is guided by experimental observations. It turns out that experiments on the class of materials investigated here are scarce. Often they do not provide a comprehensive information since only a very particular type of stress paths is examined. The idea here was to explore if there are some systematic methodologies to derive a constitutive model, having in mind a particular soil microstructure.

The objective of modelling is to derive a macroscopic or "external" relationship between stress (σ^{ext}) and deformation (ε^{ext}). However, the material components (bond and matrix –or aggregates–) provide an incremental relationship between bond strain and stress (σ^b, ε^b) and clay aggregates strain and stress (σ^M, ε^M).

The following approaches will be followed: First a relationship between strains (ϵ^{ext} , ϵ^b , ϵ^M) will be sought by invoking mass balance relationships. These relationships will be formulated in volumetric terms. It will be shown that mass balance relationships do not provide the complete answer and some additional "constitutive" assumptions have to be made at this level of model development in order to know the component strains (ϵ^b , ϵ^M) given the external strain (ϵ^{ext}). This stage of model development will produce a "partition of strains". The next step is to relate the strain components (ϵ^b , ϵ^M) with its associated stresses (σ^b , σ^M). This is solved by selecting a particular constitutive model for each of the components. The third stage is the integration of the stress components (σ^b , σ^M) into an external stress (σ^{ext}). This final stage involves also an educated guess, guided by the conceptual representation of the microstructure. Some general procedures may also be invoked (the principle of virtual work) but it may also lead to undesirable effects.

Two classes of models will be developed: Model 1 and Model 2. Model 1 is inspired by mixture theory and Model 2 is inspired by a structure of grains connected bond.

5. Conceptual representation of microstructure and modelling

Model 1



Figure 2. Conceptual representation of a bonded expansive material. (a) for Model 1 and (b) for Model 2.

The conceptual representation is given in Figure 2. It integrates two entities at macro level: bond and clay aggregates. Since aggregates are made of the stacked clay particles, a micro level is considered

which includes clay particles and microvoids inside the aggregates. Accordantly, Reference Elementary Volumes Macro (REV^{Macro}) and micro (REV^{micro}) are considered as shown in the Figure 2. Mass balance equations of clay are written over a REV^{Macro} and REV^{micro} and bond mass balance equation only at REV^{Macro}. Finally a mass balance equation of solid particles (bond and clay) are considered over REV^{Macro}. Algebraic manipulation of this mass balance equations leads to the following relationship:

$$\dot{\varepsilon}_{vol}^{ext} = c^c \dot{\varepsilon}_{vol}^{ag} + c^b \dot{\varepsilon}_{vol}^b \tag{8}$$

where c^c and c^b are clay and bond mass concentration and $\dot{\varepsilon}_{vol}^{ag}$ is the volumetric strain rate associated with the aggregates which include changes of their own volume (due to changes in microporosity) and volume changes associated with its topological configuration which affects to the macroporosity. $\dot{\varepsilon}_{vol}^b$ corresponds to the volumetric strain of bond. It includes changes in bond density and its topological configuration which also affects the macroporosity.

Equation (1) does not solve the problem because given the external strain rate, the strain rate of components cannot be identified. An additional relationship is required. For instance:

$$\varepsilon_{vol}^b = \chi \varepsilon_{vol}^{ext} \tag{2}$$

where χ is a constitutive parameter. Equation (2) specifies that a proportion of the external strain deforms the bond. Parameter χ will decreases as damage increases. Equation (2), in fact, is a constitutive relationship and it has a significant effect on the overall constitutive behaviour. Other choices are, of course, possible. They may be inspired in a conceptualization of the soil microstructure.

Model 2

The conceptual representation is shown in Figure 2 b. The bond is conceived as an structural network than partially fills the pores between aggregates and/or covers them. Three representative elementary volumes will be defined: REV^{m/micro} for clay particle at micro level, REV^{b/micro} for bond at micro level and REV^{Macro} at macro level which include the entire composite material. REV^{micro} are embedded within REV^{Macro}. Now bonds are assumed to link and hold together clay aggregates. Then, at macro level, the average velocity of bond particles are assumed to be the same as the average velocity of clay aggregates. Clay and bond mass balance equations are written at REV^{micro} and REV^{Macro} and allow to obtain the following strain partition:

$$\dot{\varepsilon}_{vol}^{ext} = \dot{\varepsilon}_{vol}^{V} + \phi^{m} \dot{\varepsilon}_{vol}^{m} + \phi^{b} \dot{\varepsilon}_{vol}^{b} \tag{3}$$

where ϕ^m and ϕ^b are the volumetric concentration of aggregates and bond respectively. $\dot{\varepsilon}^{\nu}_{vol}$ is the volumetric strain rate associated with to the changes in macrovoids, $\dot{\varepsilon}^m_{vol}$ is associated to the changes in volume of aggregates and $\dot{\varepsilon}^b_{vol}$, unlike Model 1, indicates the changes in the bond density.

Again, an additional assumption is needed to complete (3). The proposal now is to relate bond deformation and changes in macroporosity since the bonds will be deformed as far as aggregates change its configuration and they affect to the pores among them:

$$\dot{\varepsilon}_{vol}^b = \chi \dot{\varepsilon}_{vol}^V \tag{4}$$

6. Integration of stress components

The constitutive models for the expansive matrix and the quasi-fragil bond will not be described here. Pinyol *et al.* (2007) provide a short description of the two constitutive models. Consider, however the process of stress interpretation.

One possibility is to use the principle of virtual work applied to conjugate stress and strain variables. For instance, in the case of Model 2, application of the principle of virtual work leads to following stress integration:

$$\sigma^{ext} \Delta \varepsilon_{vol}^{ext} = \sigma^{M} \Delta \varepsilon_{vol}^{ext} + \phi^{b} \sigma^{b} \Delta \varepsilon_{vol}^{b}$$
(5)

But other choices are available. It may be also argued, having the microstructure in mind, that the external stress may be appropriately expressed as a direct sum of the bond and matrix stress:

$$\sigma^{ext} = \sigma^M + \sigma^b \tag{6}$$

In case of Model 1, it seemed logical to propose that the external stress may be decomposed as follows:

$$\sigma^{ext} = c^c \sigma^M + c^b \sigma^b \tag{7}$$

Again these hypothesis may be considered constitutive decisions and they have a significant impact in part on model performance.

7. Conclusions

The paper propose a methodology for building constitutive models of composite geomaterials. The methodology is assisted by some general rules, namely the mass conservation relationships for constituents. These relationships provide expressions for strain partition. However, it has been shown that they are dependent on the particular conceptualization of the material microstructure. In addition, they do no provide a complete answer to the problem of strain decomposition and some additional guided assumptions should be made. Similar comments may be made on the method selected to integrate stresses. It turns out that decisions concerning strains and stress decomposition have to be made on the basis of some representation of the material. In general the constituents (bond and matrix) cannot be directly tested. Therefore the evaluation of model performance relies on the overall model response. Available experimental programs are however limited. It is also felt that the class of natural materials which may be described by a composite approach is extremely wide and no reasons "a priori" to prefer a particular formulation seem to exist.

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