Effect of fabric on elastic properties of a lime treated clayey sand

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ABSTRACT

Soil stabilization processes usually acting only on a specific active part of the soil constituents are significantly affected by inert constituents through the microstructural fabric. Thus, computational homogenization may be used to understand this dependence to the fabric through morphological studies. The high heterogeneity and complexity of soils make this approach difficult, mainly at RVEs definition and discretization stage. We present here an integrated framework for soil homogenization allowing morphological studies thanks to an efficient RVE generator coupled with an XFEM setting for mechanical simulation. The link between these tools is the use of Level Set functions for the geometrical description of RVEs. The efficiency of this framework is illustrated with homogenizations of deformation moduli of lime treated soils with a morphological study on the effect of an active constituent properties evolution.

1. INTRODUCTION

The lime treatment of soils, as well as many ground improvement techniques, involve chemical activity between a mineral addition and some constitutive minerals of the soil [1]. The usual heterogeneity of soils implies that only a specific part of minerals are concerned by the reaction (e.g. the clay in lime treatment processes), a (large) part of the materials being unaffected. Depending on the type of solicitation (i.e. mechanics, hydraulic, thermal, ...), the evolution of the response of a treated soil emerges from the relation between active and inert constituents through the material fabric.

Beside efforts being made to understand, describe and quantify the fundamental mechanisms involved in the reactive part, there is an interest in developing models that can use those results to deduce and compare the emergent property modifications of soils having different inert content and morphology. Computational homogenization can be used for this purpose by modeling through microstructural descriptions the detailed behavior of a Representative Volume Element (RVE) under solicitation. This approach is in active development and has already been used to derive macroscopic behavior of simple microstructural material [4,12,6], mainly for mechanical solicitations. The application of this methodology to soils brings up several difficulties, mainly related the material heterogeneity.

Those difficulties may differ depending on the type of the solicitation studied and the method used for it. However, in most of the case, problems first arise when (**a**) trying to define an RVE and (**b**) discretize RVEs for numerical computations (e.g. finite element-type model). We focus here on these two points, other potential difficulties will be addressed in future works.

(**a**) Using computational homogenization in order to study the fabric role in soil improvement requires the use of a large number of RVEs with controlled morphological characteristics. Those RVEs have to fit the measurable macroscopic descriptors (i.e. grain size distribution, volume fraction, void content, ...), as well as permit generations of several RVE maintaining constant each controlled parameter among RVEs while keeping the random generation.

(**b**) Each RVE that has to be computationally tested is subject to a computation set up, including a mesh generation for finite element-type modeling. This particular step is theoretically not a problem but is practically very demanding and human-time consuming, especially in 3D. This dramatically limits the complexity and the number of RVE that can be used and consequently lowers the feasibility of a fabric study. An automated procedure of discretization should avoid this limitation and allow more exhaustive case studies.

We present here an integrated framework for generation and homogenization of large sets of soil RVEs under mechanical solicitations, allowing a morphological parameter study. This is illustrated in the context of lime treatment of clayey sand, for which the ratio clay(active)/sand(inert) is suspected to play an important role. To restrict ourselves to the two above mentioned difficulties, we study the impact of

this ratio on a homogenized deformation modulus, assuming a uniform increase of the clay's Young modulus to be representative of a lime treatment.

The present manuscript is structured in three main sections. *Section 2* presents descriptors for soil morphology that can be used to define RVEs. Two methodologies to produce sets of RVE varying the sand/clay ratio are presented. *Section 3* introduces tools used to generate such RVEs and use them in microstructural mechanical modeling. The home-developed RVE generator and the well-known XFEM method of discretization are briefly introduced. *Section 4* describes the homogenization procedure and presents obtained results.

2. FROM SOIL TO RVE DEFINITION

Introduction describes soils as multi-phase systems that can be studied and understood. This section describes soils morphology and leads to RVEs definition for our illustrating study. An RVE generator integrating the following considerations was presented previously in [9] and is introduced in *Section 3*.

2.1. Multi-phase system

Physically speaking, soils are three-phases systems, including a solid skeleton (grains and fine aggregates), water (free or adsorbed in solid phases) and air, filling the remaining spaces. In the context of soil treatment, a phenomenological description, mechanically and chemically derived is preferred. Phases are attributed to constituents based on their chemical activity within the treatment and on their structural behavior within the fabric under mechanical solicitations. The chosen description has also to be based on separable phases, to allow experimental identification of their properties. Three phases are thus distinguished for our purpose: inert grains, clayey matrix (including treatment's addition - lime -, water and air) and the macro-voids.

Inert grains are considered to be the part of the grain size distribution $\geq 2\mu$ m and may be assumed to be stable minerals which do not play any direct role on the treatment processes. The part <2µm, due to its electro-chemical properties, can be considered to be a distinct phase together with a certain quantity of lime from the treatment and micro-voids containing water and air. This phase play an important cohesive role, acting as a matrix, coating and bridging inert grains together. This clay/water/air/lime mix is considered as a continuous medium with specific properties, concentrating the evolving processes of the treatment. In mechanical modeling, the properties that should be provided for this phase depends on the cure progress. The treatment could therefore initially be modeled using a postulated or measured evolution for this lime-clay phase. Experimentally speaking, this phase is separable if the void and water content of this mix can be quantified and reproduced in testing samples. Finally, remaining spaces are the macro-void phase, which can be filled by air and/or water. It can be defined as the total porosity of the soil except the micro-voids detected in the clayey phase.

The microstructure of a soil is highly three-dimensional and there is no trivial way to find a 2D mechanically equivalent description of a given 3D sample. The mostly used 2D simplified model for grains assemblies description consist of 2D disks. But this can be used only for qualitative illustrations and mechanism analysis. Some morphological aspect concerning voids topology only emerge in 3D and the number of kinematically admissible mechanisms is also different. There is also no comparison possible in terms of volume fractions. The only available indication is the ratio between the volume of a sphere and the area of a disk of the same radius, but it is not enough to derive a 2D-3D equivalency rule for volume fractions in complex microstructures of soils.

The approach we present here can be formulated in 2D as well as in 3D, and should be used in 3D for quantitative purpose (i.e. quantitative comparison with experiments). However, we limit the present results to 2D developments for the ease of illustration and the low cost of computations. The presented results are thus by essence of qualitative nature.

2.2. Descriptors for RVE definition

The developed RVE generator is built to integrate the use of experimentally measurable parameters allowing the description of the soil microstructure in terms of the three identified phases.

(**a**) The size distribution of solid grains and voids and the volumetric constitution of soil are used to derive volumetric fractions of the three phases. The 2µm threshold is used to separate clay minerals and micro-voids from inert grains and macro-voids respectively.

(**b**) The size distribution of inert grains can be extracted from the global solid grain size distribution using the 2µm threshold. Relative sizes of grain in an assembly has a major impact on the spatial organization of the microstructure, and then on the stress path pattern under mechanical loading. It should be correctly reproduced by the generator.

(**c**) The grain shapes can be characterized and reproduced qualitatively. The generator therefore has to integrate various shapes, from the quite simple geometry of crystalline minerals to the more rounded and/or irregular shape resulting from the soil constituents history (alteration, fragmentation, rolling, ...).

(**d**) The micro-voids included in the lime-clay mix are not explicitly described in the RVE, except if it is required, by mapping the matrix properties with a density map obtained by micro-tomography, and if this density can be used in a density-dependent constitutive model. The macro-void sizes and shapes can be seen as a consequence of the compaction rate and of the spatial arrangement of grain and clayey matrix in the microstructure.

(**e**) The clay bridges morphology, especially the fraction linking effectively two grains and transmitting stresses may be an important parameter in the structural system of the fabric. The generator is built to allow these parameters to be controllable in terms of volume fraction of bridging clay, relatively to the global clay fraction. Point (**d**) and (**e**) are correlated because the morphology of clay bridges constraints the sizes and shapes of macro-voids and conversely.

2.3. Morphology of RVE for clayey sand

In this contribution, we chose to focus on the clay/sand ratio of clayey soils as the main morphological parameter to study. In terms of the assumed phases described before, this type of soil with bi-modal distribution of solid grain size is simply described as a distribution of sand grains of quasi uniform size highly-bridged by a clay matrix (*Figure 1.a*). We may use simple shapes for sand grains, as that can be observed on micrographs (*Figure 1.b*).

Figure 1: Micrograph of clayey sand. a) Clay bridge detail. [2] b) General view of microstructure (dark : clay, light grey-yellow : sand grains, white : voids) [2]

The method used for RVE generation will be introduced in *Section 3*, we describe here the RVE construction process from a morphological point of view.

The RVE construction begins with the generation of a population of grains in the RVE by LS-RSA (see *Section 3.2*), using quite simple and regular shapes and a uniform distribution of size within a moderate range (*Figure 2.a*). Then remaining areas are divided in macro-voids and clay, this operation should create the previously mentioned and illustrated clay bridges. This is performed by using the product of the two distances from a point **x** to the two nearest sand grains to impose a criteria O(**x**) of bridge presence on this point **x**. The chosen form of $O(x)$ (see *Section 3.3*) allow coating and bridging the sand grains in a single operation (*Figure 2.b*), providing moreover a tuning coefficient to adapt the bridge quantity for a given sand, macro-void and total clay quantity. This parameter is certainly not the first one to study, even if it could be of major importance, it is not directly identifiable with actual experimental observations. It is then fixed here to an intermediate value and kept constant for every RVE used.

Figure 2: Generation process for clayey sand. a) Generation of sand grain distribution, shapes mimic plane sections of quasi-regular sand grains. b) Generation of the bridging clayey matrix using distances rules.

The methodology to vary the sand/clay ratio starting from one of such RVEs is to modify it smoothly by slightly moving phase boundaries in order to obtain a set of RVEs with the same global pattern but with an evolution of the studied ratio. There are basically to ways to proceed, both are performed in the study. (**a**) From a given microstructure, move the boundary between clay and voids to increase clay fraction and keep grain fraction unchanged, decreasing the ratio sand/clay but decreasing also the macro-voids (*Figure 3)*. (**b**) From a given microstructure, move the boundary between clay and grains to increase the clay fraction, decreasing the grain fraction and keeping the macro-voids unchanged (but changing nonetheless the total void content because of micro-voids in clay) (*Figure 4*). This second procedure, preserving the void/solid ratio can be preferred but leads to "visually less realistic" microstructures for low sand/clay ratio. Moreover, under the same compaction energy, real samples with different sand/clay ratio will not be compacted to the same density, which is more reflected by the (**a**) case. It should be mentioned that strategies (**a**) and (**b**) do not allow varying the sand/clay ratio within the same range.

Figure 3: Result of procedure (a) on a random sand grain distribution. Volume fraction of these RVE are reported in the Table 1, under label step 1, 3 and 5 for right, center and left RVE respectively.

Figure 4: Result of procedure (b) on a random sand grain distribution. Volume fraction of these RVE are reported in the Table 2, under label step 1, 3 and 5 for right, center and left RVE respectively.

The RVE size should take part of the RVE definition, and this after having performed a variability study on homogenized quantity for several RVE sizes. The chosen size should be large enough to minimize variations on homogenized quantities but being small enough to be computed as discussed in [3]. Given the illustration purpose, this size dependency study is not performed here.

3. FROM RVE DEFINITION TO MICROSTRUCTURAL MODELING

This section gives an overview of different computational tools used to build the homogenization framework. *Section* 3.2 and 3.3 concern the RVE generator we develop, which is described more in details in [9]. *Section* 3.4 introduces the well-known XFEM methodology, largely described and illustrated in [10,7,5]. Those two methodologies use the Level Set functions as a geometrical tool which is the topic of *Section* 3.1.

3.1. Geometrical representation

The morphologically controlled random generation and the automated discretization of defined RVEs require several highly complex and cumbersome geometrical operations. The Level Set formalism [8] offers the possibility to handle heavy geometries with a fixed number of data which do not depend on the geometry complexity. The use of Level Set functions here is also highly motivated be the existence of XFEM techniques allowing the use of these functions as geometrical input for computations instead of meshes.

In 2D, Level Set functions are functions of x defining implicitly a planar curve φ by the solution of $\varphi = LS_{0}(x) = 0$ (1)

Various functions can be used as Level Set to define interfaces in a RVEs but the signed distance to the defined interface offers additional opportunities. Functions such as the first and second nearest neighbor function, denoted here $LS_1(x)$ and $LS_2(x)$ (*Figure 5*) can be constructed from signed distance functions of grains of a distribution and are extensively used as map by the RVE generator during the grain distribution stage. The clay bridges generation uses distance rules to define morphological quantities measured trough the microstructure by combinations of distance functions.

Figure 5: Distance functions of an arbitrary distribution of grains. <i>a) $LS_1(x)$ *b*) $LS_2(x)$.

3.2. Generating a grain distribution

The generation of the grain distribution is performed by a Level Set controlled Random Sequential Addition (LS-RSA). This method adds grains one by one at random locations constrained by a criterion in terms of distances to previously added grains. For example, overlapping of grains is avoided by imposing the new grain to be added at more than a minimal distances related to the grain size. Other distances criteria in terms of neighboring distances can be used to control the global spatial organization of the generated microstructure. Actually, generating RVEs with a large quantity of grains with highly distributed sizes, enforcing a given density in most of the case require to impose the neighboring distances to be relative to the particle sizes or particle densities to achieve homogeneous and random packings. Otherwise, generation of RVEs with very high fraction of grains require an optimal spatial organization minimizing all inter-grain distances.

Functions $LS_1(x)$ and $LS_2(x)$ are maintained during the RSA procedure on a regular fine grid on the RVE and the random generation position is restricted to points of this grid respecting imposed criteria. Different criteria are illustrated in *Figure 6* and are briefly described here. (*Figure 6.a*) Non-overlapping criterion, only points satisfying $LS_1(x)$ > R are accessible to the location generation for a grain of radius R (red area). (*Figure 6.b*) Minimizing neighboring distances, only points which combines smaller values of $LS_1(x)$ and $LS_2(x)$ in addition to pass the non-overlapping criterion are selected. (*Figure 6.c*) Specific value of neighboring distances can be used to reach a given grain density in an homogeneous packing.

Figure 6: Criteria for the random position generation restriction.

The Level Set description of the grain boundaries offers the possibility to modify their shape and size after the generation by directly acting on their Level Set. For example, the (**b**) procedure explained in *Section 2* adds iteratively an increasing constant value to the Level Set of each grain. This causes the inward movement of grain boundaries and the decrease of their volume without topological change of their shapes.

3.3. Generating clay bridges

Level Set functions of all the grains in the generated distribution can be used to construct a global descriptor of the microstructure. The generation of bridges can be formulated in terms of neighboring distances by placing bridges "where two particles are close to each other". This expression can be quantified and expressed in terms of functions built on sums or products of previously introduced LS₁ and $LS₂$ functions. Several approaches are available but are not discussed here. The following simple function is used :

 $O(x) = LS_1(x).LS_2(x)^{k}$

 $-t$ (2) to extract the interfaces separating macro-voids and clay from $O(x) = 0$. The exponent κ is the tuning coefficient mentioned in *Section 2* and *t* is the parameter used to vary to resulting clay volume fraction without changing the bridging morphology in procedure (**a**).

It should be mentioned here that this equation can be also iteratively solved to find *t* when an imposed resulting volume fraction is required from experimental evidences. We use the direct resolution here by imposing *t*, which causes the slight variations observed in clay fraction when the same *t* is used to built clay bridges on different random grain distributions. The measured amplitude of those variations for RVEs used in the results are given for information (see *Section 4.1*).

3.4. Using XFEM to compute RVE mechanical responses

The automated discretization for finite element computation of RVE for mechanical modeling uses an XFEM setting [10,7]. This allows the use of one single regular mesh for the discretization of many large RVEs sets provided that Level Set functions are available to define grains and voids geometries of each RVEs. Level Set functions given by the generation process are used in the XFEM procedure to construct additional shape functions representing deformation modes related to material discontinuities within heterogeneous finite elements. Those shape functions, called enrichment, are directly derived from the Level Set functions and used to introduce the geometry of grains and voids in the mechanical computation independently of the used mesh (*Figure 7)*.

Figure 7: Vertical strain distribution under vertical compression computed with regular meshes and XFEM. Red stands for low and blue for high compressive strain value. a) A stiff inclusion in a soft material. b) A void in a soft material.

The implemented XFEM setting is based on tri-linear elements and the enrichment used is the $F²$ enrichment presented in [7]. The multi-enrichment strategy proposed in [11] is used to resolve touching grains situations. Some examples of XFEM computation are given in *Figure 8*.

Figure 8: Vertical strain distribution under vertical compression of RVEs from the procedure (a) and (b) computed with XFEM. The used clay Young modulus is 20 MPa, see section 4 for other parameters. a) Procedure (a), step 2. b) Procedure (b), step 5.

4. FROM MICROSTRUCTURAL MODELING TO HOMOGENIZATION

As an illustration of the introduced framework, we proceed now to elastic homogenization of RVEs applying on them an increase of the local clay Young modulus to roughly simulate a lime treatment.

4.1. Homogenization set up

An *RVE set* is a set of RVEs produced from the same sand grain distribution with different sand/clay ratio, produced by the (**a**) or (**b**) procedure. Each RVE of a *set* is subsequently homogenized for different increasing Young moduli for the lime-clay matrix. Finally several *sets* are generated by both procedures to be aware of the dispersion linked with the randomness of RVEs and to be able to evaluate averaged quantities. We suppose here an homogenous soil so that each *RVE set* is generated with the same governing parameters, the randomness originates only from the initial sand grain distribution. One could be interested in including a natural variability of macroscopic soil descriptors trough RVEs generations. It is not done here even if slight variations of volume fraction are observed through RVEs at a same level of procedure (**a**) or (**b**). Theses variations are linked with a detail of the generation method and can be avoided as explained in *Section 3.3.*

Homogenization of deformation moduli is performed by modeling uni-axial compressions on RVEs in oedometric conditions and within the elastic domain of materials. Such homogenized moduli are thus not Young moduli. They should be seen as compressibility (oedometric) moduli, having only a physical meaning for episodes of slow uniform loadings of large areas on highly surconsolidated soils. We consider that voids are water saturated and we model the result of stabilized deformations under effective stresses after drained compressions by ignoring water pressure contributions in computations. A 2D plane strain assumption is used. These simple conditions are chosen for the simplicity of the mechanical model required. Enlarging the domain of solicitations (e.g. by loading until plasticity and failure) brings specific difficulties that cannot be aborted here.

30 *RVE sets* of type (**a**) are generated with a sand grain volume fraction of 0.7±0.01 and with a clay volume fraction increasing from 0.106±0.008 to 0.256±0.01. This correspond respectively to macro-void volume fractions from 0.194±0.012 to 0.044±0.008 and average sand/clay repartition from 86.8 / 13.2 % to 73.2 / 26.8 %.

25 *RVE sets* of type (**b**) are generated with a macro void volume fraction of 0.089 ± 0.01 and with clay volume fractions increasing from 0.189±0.01 to 0.499±0.02. This correspond respectively to sand grain volume fractions from 0.722 ± 0.01 to 0.412 ± 0.02 and average sand/clay repartition from 79.2 / 20.8 % to 45.2 / 54.8 %.

Each RVE is homogenized with increasing value of clay's Young modulus from 0.1 to 40 MPa to represent locally the lime treatment effect. The clay's Poisson ratio is fixed to 0.3 and the sand grains use quartz crystal values, 100 GPa for Young modulus an 0.1 for Poisson ratio. The two following table summarize the *RVE sets* composition :

Table 1: Average volume fraction of RVEs from procedure (a)

	Clay	Macro-voids	Sand	Sand/Clay
Step 1 :	0.106	0.194	0.700	$86.8 / 13.2 \%$
Step 2:	0.142	0.158	0.700	$73.2 / 16.8 \%$
Step 3 :	0.169	0.131	0.700	$80.5/19.5\%$
Step 4 :	0.210	0.090	0.700	$76.9 / 23.1 \%$
Step 5 :	0.256	0.044	0.700	$73.2 / 26.8 \%$

4.2. Results presentation

Homogenized moduli are plotted here versus the clay (**I**) Young modulus (figures on the left) or (**II**) volume fraction (figures on the right). Graphs (**I)** illustrate the effect of our idealized treatment. The different blue curves are constructed by averaging and linearly interpolating the results obtained from all the RVEs having the same clay volume fraction and homogenized with the same clay modulus. The transition from dark to light denotes the increase of the clay volume fraction. Graphs (**II**) invert the role of clay Young modulus and volume fraction, the transition from dark to light for the reds curves denotes then an increase of the clay Young modulus. The value of the clay Young modulus of each red curve of a (**II**) graph can be read in the corresponding (**I**) graph and conversely.

4.2.1. Case (a)

These first computations exhibit clearly a linear dependency of the homogenized modulus with the clay volume fraction (*Figure 9.II*). The studied volume fraction range is to sharp to conclude, but this means that in this domain of behavior, increasing the clay volume fraction by expanding an existing clay fraction does not modify the microstructural system but simply linearly increases its stiffness. The same results plotted in terms of relative increase of homogenized modulus degenerate in a single curve due to this linear behavior and this is not plotted here.

Figure 9: Results of case (a) in terms of homogenized moduli.

4.2.2. Case (b)

Computations of RVEs of case (**b**) reveal a different behavior (*Figure 10*). First here, the homogenized modulus decreases for an increase of the clay volume fraction because the added clay replaces a volume of grain which is the stiffer material. This relation is however not strictly linear anymore, note that the studied range of clay volume fraction more significant in this case.

Figure 10: Results of case (b) in terms of homogenized moduli.

These results are clearly in agreement with intuition. Actually, trends of set (**a**) reflect probably more the increase of solid fraction that anything else while those of the set (**b**) reflect the decrease of the grain fraction, the main stiffness source. But this time, homogenized modulus relative increase shows a dependence to the morphology (*Figure 11.I*). The rate of increase of homogenized moduli is lower for low clay contents than for higher contents, there is a modification of the microstructural system. The increase of the inter-grain distances (see *Figure 4*) correlated to the clay volume fraction increase in the (**b**) procedure is a good potential explanation of this.

Figure 11: Results of case (b) in terms of homogenized modulus relative increases.

The variability on homogenized quantities related to RVEs size is well appreciated thanks to the large number of homogenized RVEs. This variability is substantial but does not interfere for trends extraction and should not be an inconvenient for engineering usage of this kind of results.

5. DISCUSSION

A methodology to apply homogenization technique for simple mechanical loading on soils is presented. The influence of a lime treatment modifying the clay properties in a specific soil can be studied by providing this information at the microstructural scale. The microstructural description is fine enough to distinct inert and active phases and large enough to be averagely representative of an macroscopically homogeneous soil. A simple morphological parameter is studied, the ratio sand/clay of a clayey sand and the results seem to agree with intuitions.

However, this 2D study cannot be properly compared to experimental results. First, because 2D volume fractions used in this study cannot be linked with experimental sample measured 3D composition. Furthermore, neither the (**a**) nor (**b**) procedures lead to RVE set compositions which match with sample set compositions usually used in experiments and because those procedures involve other parallel modifications in the microstructures. Using proctor optimum in experiments leads to intermediate but not predictable situations. For a 3D experimentally reliable study, *RVE sets* should be produced to respect exactly the composition of a prepared sample set used for experiments. This require to be able to measure the clay phases micro-porosity to deduce the macro-voids content from the global porosity. This can be performed by mercury absorption or X-ray tomography by measuring the local clay density.

This study is only an example, a lot of geomaterials and constituent evolutions can be analyzed through this framework. More complex mechanical behaviors and loading can be analyzed with plasticity and density dependent constitutive models for clay fractions while damage models should be pertinent for highly cemented phases (i.e. at long curing time of a lime treatment). Any large or localized deformation occurring during loading on such RVEs leads to the inefficiency of the presented framework that should be adapted for such situations. However, this framework can also be used for various problem including heat conduction, electrostatic potential repartition, seepage,

From a strict computational point of view, this contribution demonstrates the efficiency of the coupling between LS-XFEM discretization and the LS-RSA generator. This particular efficiency is absolutely required to perform this kind of multi-scale morphological study. The 1650 computations of this study require around 60 hours on 12 CPU but only a light afternoon of human-time for preparation.

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