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Numerical modelling of the swelling of clayey geomaterials: A comparative study between Barcelona Basic model (BBM) and a multiscale approach

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ABSTRACT: Clay swelling occurs at diffrent scales and is governed by two phenomena: crystalline and osmotic swelling. In this work, we propose a comparative study between two numerical models. The first one is a multiscale constitutive law, based on a phenomenological approach conducted to formulate the different interactions that occur in the interlayer space with respect to the disjoining pressure (crystalline swelling) and the interparticular porous space to account for capillarity effects. The model is freshly developed and implemented in Code_Aster Finite Element software for hydro-mechanical coupling and showed a good consistency with experimental results. The second model is the highly acknowledged Barcelona Basic model already existing in Code_Aster. BBM model is already validated in the literature showing a good tendency with the experimental results. The idea of this paper is to compare between the two models as they have both reproduced the real swelling behaviour of clayey geomaterials comparing to the experimental results. To this aim, we will be focusing on the swelling mechanism existing in constant-volume conditions in terms of swelling pressure.

Keywords: Constitutive modelling, BBM model, Clay swelling, Disjoining pressure, Homogenization

1 INTRODUCTION

Swelling of clay rocks gained throughout time a wide interest as they are the main hosting rocks of radioactive wastes (namely, Boom clay in Belgium, Opalinus clay in Switzerland, Callovo-Oxfordian argillite in France). This led rock mechanics scientists to conduct important works concerning these materials. In numerical terms, several models chiefly considered clay rocks as double-structured materials considering nanoscopic and microscopic porosities (Cariou et al., 2013, Eghbalian et al., 2022). This approach is consistent with the observed microstructure of these clay materials.

As for Barcelona Basic Model developed by Alonso et al., (1990) it has been widely used to describe the behaviour of clay geomaterials (bentonite, clayey soils, etc) and hence showed a good tendency while comparing to experimental results (D'onza et al., 2016).

The overall model based on Cariou et al., 2013; is established using the upscaling of the nanoscopic elasticity law that governs the clay particle through the Levin theorem. It links the macroscopic stress tensor to strain tensor by means of the homogenized elasticity tensor and the different interactions (interlayer disjoining pressure and interparticular interactions).

This paper aims to compare the two constitutive models and present some of the outcomes of the previously developed model for further advanced modelling applications in both soils (shallow foundations on clay soils <1.5-2m of depth) and rock mechanics (namely self-sealing of clayey rocks). Furthermore, we will present the theoretical aspects of the model with a brief reminiscent of BBM model and compare the different aspects of the formulation afterwards, we will highlight the main results of the comparative study.

2 THEORETICAL DEVELOPMENT

2.1 *Developed multiscale approach*

The multiscale developed approach previously developed (Mhamdi Alaoui et al., 2023) is given in the overall mathematical formulation of Equation (1) in tensorial notation, is based on the upscaling previously performed in Cariou et al., (2013). It relates the macroscopic strain tensor $\boldsymbol{E}$ to the macroscopic stress tensor $\delta\boldsymbol{\Sigma}$ using a new defined homogenized elasticity tensor $\mathbb{C}^{hom}$ and other parameters mainly the interparticular equivalent pressure P_m^{eq}, the disjoining pressure π_g, the liquid pressure p^l using the coupling parameters of Biot tensor $\boldsymbol{B}$. Each parameter will be discussed separately in the upcoming part of the paper i.e., the disjoining pressure and interparticular equivalent pressure.

$$\delta\boldsymbol{\Sigma} = \mathbb{C}^{hom}\colon\boldsymbol{E} - \left(\left(\delta p^l + \delta\,\pi_g\right)(\boldsymbol{1} - \boldsymbol{B}) + \delta P_m^{eq}\boldsymbol{B}\right) \tag{1}$$

$$\mathbb{C}^{hom} = \mathbb{C}^{dr}_{mt} + \frac{\varphi_{inc}}{1-\varphi_{inc}}\mathbb{P}^{-1} \quad (2)$$

φ_{inc} is the concentration of inclusions (non-clay minerals: quartz, etc) within the material.

The elasticity tensor of the clay matrix $\mathbb{C}^{dr}_{mt}$ is established using the Mori-Tanaka homogenization scheme that showed good accuracy on reproducing the elasticity parameters comparing to experimental measurements (Abou-Chakra Guéry, 2010). The mathematical formulation of the proposed homogenization writes for drained conditions:

$$\mathbb{C}^{dr}_{mt} = (1-\varphi)\mathbb{C}^{iso}_{par}:\left[(1-\varphi)\mathbb{I}+\varphi\left[\mathbb{I}-\mathbb{P}:\mathbb{C}^{iso}_{par}\right]^{-1}\right]^{-1} \quad (3)$$

φ stands for the porosity within the clay matrix.

In Equation (2-3) $\mathbb{P}$ is the Hill tensor established for a spherical inclusion immerged in an isotropic matrix and $\mathbb{C}^{iso}_{par}$ the elasticity tensor of the clay particle with respect to the particle stiffness. Both tensors are calculated after conducting an isotroropization procedure (Bornert, 2001). Once the calculations are performed, another isotropization step is conducted to extract the elasticity parameters mainly (k^{dr}_{mt}, μ^{dr}_{mt}) as the compressibility and shear moduli of the clay matrix, these last depends on the elasticity parameters of the clay layer and other parameters of the clay particle (viz. porosity within the clay particle and the normal stiffness of the clay particle).

Similarly, we proceeded to establish the Biot tensor $\boldsymbol{B}$ considered as the first hydro-mechanical coupling parameter. Once again, we use the Mori-Tanaka homogenization scheme and isotropization algorithms to formulate the tensor. The latter reads for drained conditions:

$$\boldsymbol{B} = \mathbf{1}:\left(\mathbb{I}-\left[\mathbb{C}^{iso}_{par}\right]^{-1}:\mathbb{C}^{dr}_{mt}\right) \quad (4)$$

Figure 1. schematizes two parallel clay layers, these last, regarding the charge deficit that reigns in the interlayer space, attracts cations in water molecules; subsequently, the disjoining pressure starts developing in the interlayer space along with the water pressure as the clay particles are always saturated. It is formulated in our case by using a phenomenological approach that assembles all the interactions that chiefly governs the interlayer space.

The disjoining pressure takes into account three different interactions $\pi^e_d(h, c_i)$ as the electrosatic repulsive component of Poisson-Boltzmann equation responsible for the 4W hydratio state (four water layers accumulated in the interlayer space: interlayer osmotic swelling), π^{vdw}_d van-der-Walls attration forces as the attrcative constituent of π_g, hydration forces through π^s_d main mechanism accountable for 1-2W hydration states of crystalline swelling (Gonçalvès et al., 2010).

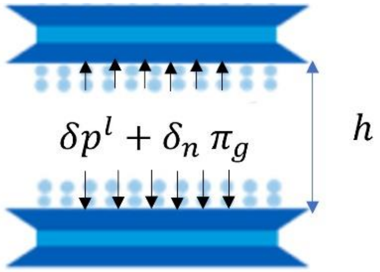

Figure 1. Phenomenological description of the clay particle

. The overall formulation of the disjoining pressure gives:

$$\pi_g = \pi^{vdw}_d - \pi^e_d - \pi^s_d \quad (5)$$

$$\pi^e_d = \frac{1}{CEC}\sum_{i\epsilon I} 2exc_i c_i N_A kT(cosh[u_i]-1) \quad (6)$$

$$\pi^{vdw}_d = \frac{A_h}{3\pi}\left(\frac{1}{(h)^3}+\frac{1}{(h+2t)^3}-\frac{2}{(h+t)^3}\right) \quad (7)$$

$$\pi^s_d = \kappa.\exp\left(\frac{-0.5h}{\lambda}\right) \quad (8)$$

Table 1. Parameters of the disjoining pressure

$\boldsymbol{CEC}$	Cation exchange capacity of the mineral
$\boldsymbol{exc_i}$	Exchangeable cation capacity
$\boldsymbol{I}$	Interlayer cations
$\boldsymbol{c_i}$	Molar concentration of the cation
$\boldsymbol{h}$	Interlayer spacing
$\boldsymbol{t}$	Thickness of the clay sheet
$\boldsymbol{N_A}$	Avogadro number
$\boldsymbol{u_i}$	Electrical potential at the mineral surface
$\boldsymbol{T}$	Temperature
$\boldsymbol{k}$	Boltzmann constant
$\boldsymbol{\kappa-\lambda}$	Material parameters

The geometry of the interparticular pores is difficult to be characterized, most of the experimental techniques use different assumptions to simplify the task. In this developed multiscale approach, we assume that interparticular pores have a spherical shape, and regarding the non-saturated state of the material, these pores are thus, either saturated with liquid (water) or gas. The threshold that discriminates this possibility is noted r^* and is established using Laplace law. Consequently, the interparticular pores are henceforth, subjected to one equivalent pressure P^{eq}_m that account for capillarity and interfacial effects, with respect to the pore size distribution (PSD) that is assumed better fitted with Gaussian distributions. The formulation of P^{eq}_m gives:

$$P_m^{eq}(p_c) = \frac{1}{\xi}(\sum_i \int_{r_m}^{r^*}(p^l - \frac{2\gamma^{sl}}{r})\alpha^i(r)dr + \sum_i \int_{r^*}^{r_M}(p^g - \frac{2\gamma^{sg}}{r})\alpha^i(r)dr) \tag{9}$$

$$r^* = \frac{2\gamma^{lg}}{s} \tag{10}$$

Table 2. Parameters of the interparticular equivalent pressure

s	Suction
$\boldsymbol{p^l}$	Liquid pressure
$\boldsymbol{p^g}$	Gas pressure
$\boldsymbol{\alpha^i}$	Gaussian distributions
$\boldsymbol{\xi}$	Total volume of interparticular pores $\int_{r_m}^{r_M}\alpha(r)dr$
$\boldsymbol{\gamma^{sl}}$-$\boldsymbol{\gamma^{sg}}$	Surface tension solide-liquid, solid-gas respectively
$\boldsymbol{r_m}$-$\boldsymbol{r_M}$	Minimum and maximum interparticular pore radius

This definition given to the interparticular pressure implicitly defines a new intrinsic material parameter, it is the water retention curve (WRC) of the material. Regarding Equation (9), the WRC links the saturation degree S_l through the Gaussian distributions to suction, it is the volume of pores saturated with liquid divided by the total volume of inerparticular pores ξ. This defintion will be the first parameter to be compared to the formulation used for the BBM model.

$$S_l(p_c) = \frac{1}{\xi}\sum_i \int_{r_m}^{r^*}\alpha^i(r)dr \tag{11}$$

After all the formulation is conducted, the numerical model is then implemented in Code_Aster (EDF) as a new multiscale definition of the effective stress principle governing the coupled chemo-hydromechanical processes of clay materials.

2.2 Barcelona Basic Model (BBM)

The hydromechanical swelling behaviour of clayey geomaterials has been widely studied in both multi-physical and multiscale frameworks. Accordingly, BBM model (Alonso et al., 1990) showed good accuracy while compared to experimental tests and captures the main characteristics of the behaviour of unsaturated soils. It is based on a modified formulation of Cam-Clay model.

In isotropic stress conditions, BBM stipulates that both changes in net stress p and suction s contribute to changes in the volumetric elastic strain through Equation (12) given in incremental form where κ is the elastic swelling coefficient and κ_s elastic swelling coefficient for a suction decrease.

$$d\varepsilon_v^e = \frac{\kappa}{1+e}\frac{dp}{p} + \frac{\kappa_s}{1+e}\frac{ds}{s+p_{atm}} \tag{12}$$

The model captures two major aspects: during a hydration phase, the soil swells at small pressures and collapses for high pressure; during a desaturation (suction increase) that induces irreversible strains, consolidation pressure increases. Under these assumptions two curves help define the yield surface: LC (Loading collapse) and SI (Suction increase). The latter is a linear function of elastic limit of suction. As the LC formulation it gives:

$$\frac{p_0}{p^c} = (\frac{p_0^*}{p^c})^{\frac{\lambda(0)-\kappa}{\lambda(s)-\kappa}} \tag{13}$$

The compressibility decreases with suction through $\lambda(0)$ and is formulated as:

$$\lambda(s) = \lambda(0)[(1-r)\exp(-\beta s) + r] \tag{14}$$

Generally, for hydro-mechanical coupling, van Genuchten, (1980) WRC is highly acknowledged in the literature. It is a formulation that is based on isothermal conditions for unimodal bell-shaped PSD.

$$\frac{S_l - S_r}{1-S_r} = \frac{1}{[1+(\frac{s}{p_r})^n]^{1-\frac{1}{n}}} \tag{15}$$

This formulation exhibits 3 material parameters S_r residual saturation in non-connected porosity, p_r the capillary pressure corresponding to the residual saturation, n as a material parameter. This formulation is generally coupled with Mualem expression for the relative permeability. In this study, the same formulation is used to formulates the relative permeability for the developed multiscale approach.

BBM has 10 material parameters that needs several experimental tests to be determined. The lack of knowledge of these parameters didn't favourite the dissemination of the model among the researchers. In this context, D'onza et al., (2016), performed a serial of fitting tests considering experimental results for different test with different loading paths on a Spanish clayey soil. This benchmark study provided by the authors was of good help to perform the comparative study.

3 COMPARISON AND DISCUSSION

First let us compare the WRC imposed for each calculation test. VGM parameters already exists in D'onza et al., (2016). Whereas for the developed approach, no such parameters are available to fit the real PSD. To overcome this issue, as the initial suction and the initial S_l are available; the fitting parameters of the WRC are chosen in a way to clearly reproduce the initial states.

The parameters of the WRC are given in Table 3 and Figure 2. describes the observed results.

Table 3. Parameters of the WRC for the developed approach and van Genuchten (μ: is the mean, σ the standard deviation, ω is the weight of the Gaussian distributions).

WRC	Parameter	Values
Gaussian	μ_1	1 µm
	σ_1	0.1 µm
	ω_1	0.3
	μ_2	0.15 µm
	σ_2	0.05 µm
	ω_2	0.7
	r_m	0.1 µm
	r_M	0.1 mm
VGM	p_r	200 kPa
	n	1.53
	S_r	0

BBM is already implemented in Code_Aster, and its implementation has been already validated through different tests.

The authors also reproduced with the Code_Aster implementation version of the BBM model different tests to ensure its pertinence and relevance with comparison to the available experimental results and other existing versions in the literature.

The results will be given to compare the swelling behaviour of the clay geomaterial using the two constitutive laws, the latter are indeed different in terms of the formulation. they, however, can bring comparable results for different quantities and good insight on the overall swelling behaviour.

That being said, the comparison of both models is conducted by reproducing a constant-volume swelling test in new testing conditions not reported in D'onza et al., (2016) as the loading paths are adapted to be conducted also for the multiscale approach detailed hereinbefore. As shown in Figure. 3 the sample is cylindrical (h=70 mm, d=17.5 mm) and the modelling is conducted in axisymmetric conditions.

The mesh is considered uniform with 25x25 elements of 8 nodes quadrangles of P2P1 type i.e., linear interpolation for fluid pressures and quadratic interpolation for displacements. The sample is subjected to an initial isotropic confining pressure of 10 kPa. The test involves a saturation by flushing through, assuming a suction decrease from the initial imposed suction of 8 kPa occurring in 1000 seconds.

Material properties are taken based on a fitting study of tests SAT-1 and TISO-1, values are different from those reported in D'onza et al., (2016) as the authors in the latter, fitted other tests in addition to those mentioned above (see Table 4).

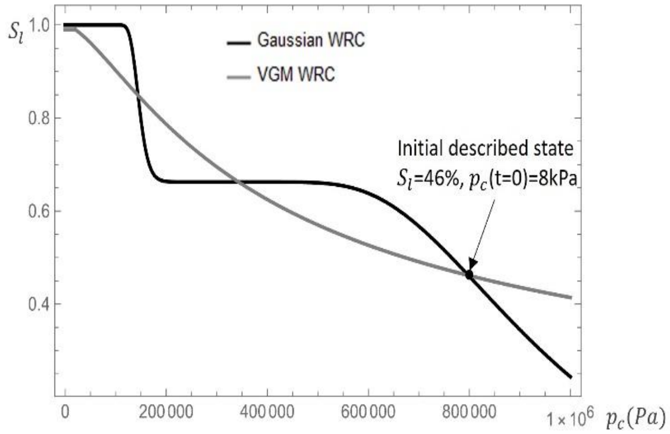

Figure 2. Comparison of the two defined WRC

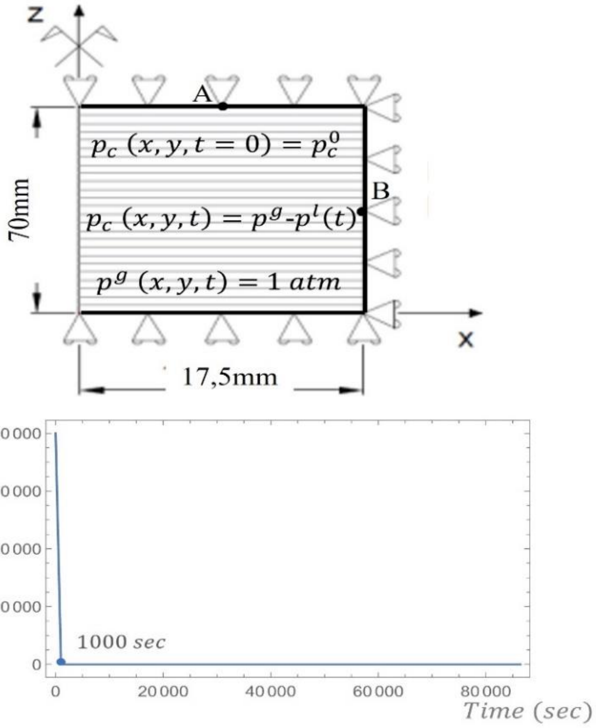

Figure 3. Geometrical and boundary conditions of the test (Modified after Gramegna et al., 2020)

Table 4. Parameters of the BBM used in this study.

κ	Elastic compressibility coefficient for changes in mean net stress	0.0012
$\lambda(0)$	Slope of the saturated virgin consolidation line	0.08
r	Parameter defining the minimum soil compressibility	1.1
β	Parameter controlling soil stiffness	10^4 kPa^{-1}
κ_s	Elastic compressibility coefficient for changes in suction	0.005
p^c	Reference pressure controlling the loading collapse (LC) curve	5.10^{12} Pa
p_0^*	Preconsolidation pressure of the saturated state	90 kPa

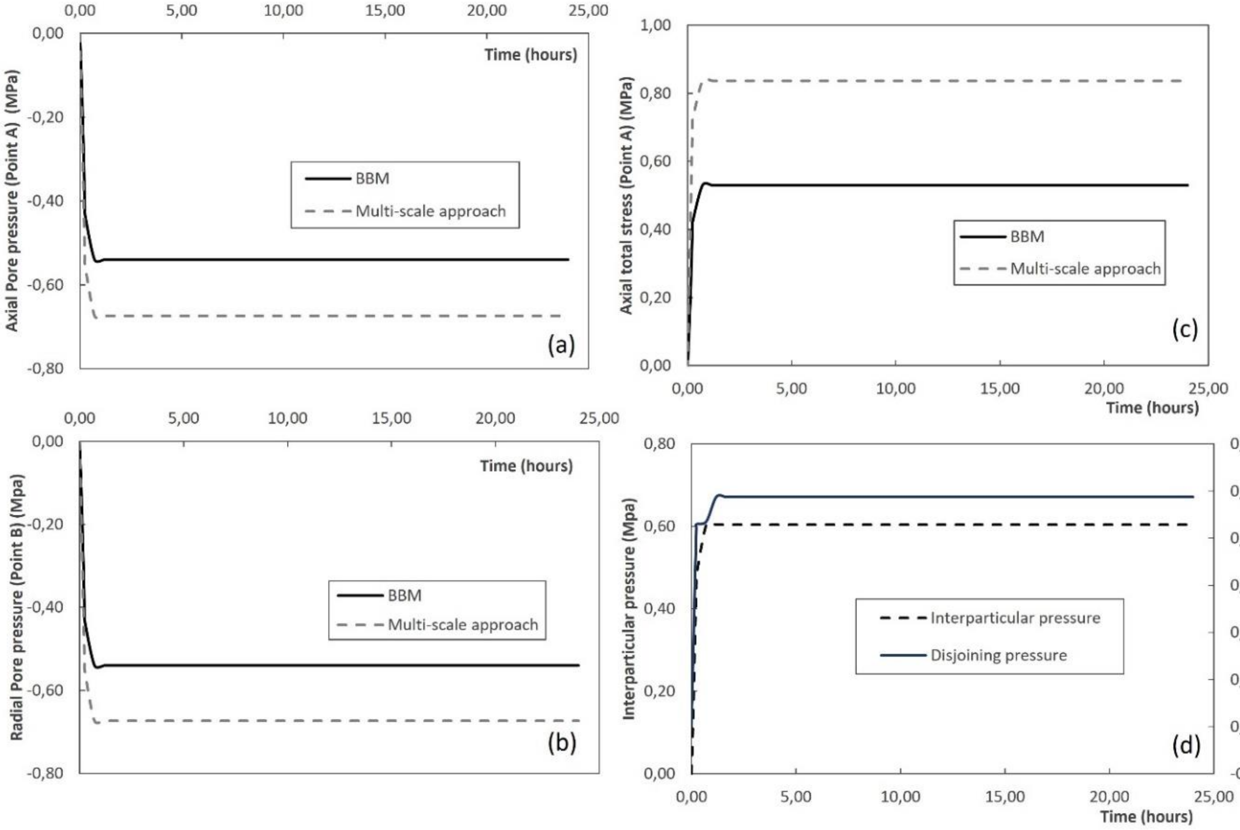

Figure 4. Calculation results for both BBM and the developed multiscale approach. (a) axial pore pressure (b) Radial pore pressure (c) Total stress in the axial direction (d) results for the disjoining pressure of Equation 5-8) and the equivalenting interparticular pressure in Equation (10)

In Figure 4(a) and 4(b) that apprehend the pore pressure, it is worth noting that the pore pressure for the developed multiscale approach is formulated using Equation (1) through $\left(-\left(\delta p^{l} + \delta\,\pi_{g}\right)(\mathbf{1}-\boldsymbol{B}) - \delta P_{m}^{eq}\boldsymbol{B}\right)$; as for the BBM the pore pressure of the model is formulated using the average pore pressure: mean of liquid and gas pressures pondered with the degree of saturation of each phase. The results showed that for all the given curves the BBM tend to reduce the swelling potential of the sample this is mainly due to the plastic threshold that intervenes to describe the collapse of the soil and hence a decrease of the swelling potential. Whereas the formulated multiscale approach gives a swelling potential more important.

From a kinetical perspective, no major differences are noticeable for both models. While comparing results of the component of the pore pressure of the multiscale approach, one can notice that the major contribution is given through the interparticular equivalent pressure P_{m}^{eq} that is formulated using capillarity and surface tension effects. In fact, since clay particles are always in a saturated state, no major changes can occur in term of water intrusion to the interlayer space, the only evolution of the disjoining pressure can mainly be attributed to the changes of pressure at the edges of the clay particles, this can change relatively the interlayer spacing and consequently, the pressure in between the clay layers. This reverts us to point out, that the WRC parameters through the Gaussian distribution is a vital parameter for robust modelling. This requires a detailed characterization of the porous space through advanced experimental approaches (i.e., Matskova et al., 2017) where authors combined mercury intruded porosimetry (MIP) and innovative gas adsorption experiments. Contrary to D'onza et al., (2016) where the PSD is provided only using MIP data.

Calculation results for the degree of saturation (Figure 5) reproduced very well the kinetics described in the WRC through the smooth saturation noticeable in the VGM WRC and the stepwise saturation of the interparticular pores recognizable through the Gaussian distributions (Figure 2) (i.e., saturation of smaller pores at a first stage and saturation of larger pores and so on). Especially for the first calculation times that is due furthermore to the hydration conditions that is relatively high and to the intrinsic permeability of the soil 9.10^{-16} m^{2}. This stepwise trend also impacted the induced forces at the edges of clay particles where a noticeable effect on the disjoining pressure was noticed: an increase in the interparticular equivalent pore pressure induced an increase in the disjoining pressure in repulsive regime.

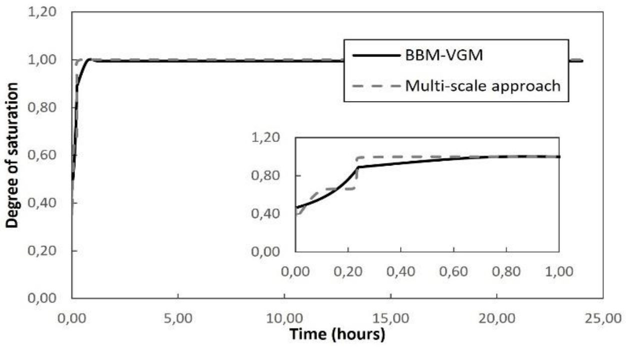

Figure 5. Evolution of the degree of saturation for both BBM and the developed approach.

4 CONSCLUSION AND PROSPECTS

This paper presented a comparative study in terms of calculation results for both the highly acknowledged BBM and a multiscale approach, some of the outcomes of this approach where also briefly detailed. In fact, both the models do not take in consideration the same modelling aspects: BBM is based on an elasto-plastic approach that describes pertinently the swelling and collapse of clayey geomaterials and mostly soils, the developed multiscale approach, however, approaches with great description, the importance of the physical interaction occurring in the porous space of clays at different scales. Therefore, the comparative study, solely looked into the swelling behaviour of the clay material in constant-volume conditions with both models.

A complete and robust comparison is still to be carried out. Being said that, the developed multiscale approach can be improved to take into account not only the non-linear poro-elasticity from the nano-scale of the clay particle as a start of the upscaling procedure, but also a plastic strain first at the macro-scale of the sample as a first step and adding subsequently the different aspects typically the formation of other clay particles while increasing the saturation: plasticity at the nano-scale. What is more, future work will account for the anisotropy of the material at macro-scale. Finally, the present work confirms the paramount importance of accurately characterizing the pore size distribution of the clayey materials.

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