Multiscale modelling of rock behaviour around underground works with an insight of microstructural characteristics influence

Benoît Pardoen
University of Lyon, ENTPE, LTDS, France

Christos Mourlas
University of Lyon, ENTPE, LTDS, France

ABSTRACT: Rock behaviour conditions the stability of deep underground exploitations. The excavations generate deformations, damage, and fractures in the surrounding rock. At engineering scale, phenomenological constitutive models are often considered; however, macroscale behaviour takes its origin from small-scale properties. Their influence on material deformations and damage across scales remains complex. Therefore, the behaviour of a clay rock is modelled at two scales. The excavation and damaged zones around galleries are reproduced at large scale. The excavation-induced fractures are modelled with shear bands. The approach is enriched with microstructural characteristics of mineral inclusions and clay matrix. The material mesostructure and behaviour are embedded in a representative elementary volume. A double-scale numerical framework (FEM×FEM) with computational homogenisation relates small- and large-scale behaviours, as deformations and failures. The damage and cracking developments at micro/meso scales allow to predict macroscale shear banding. The results highlight the possibilities of double-scale computing to predict underground structure behaviour.

Keywords: Damage, shear failure, double-scale modelling, microstructural characteristics, excavation.

1 INTRODUCTION

The long-term management of high-level nuclear wastes is envisaged by deep geological repository. Low-permeability clay rocks are considered as favourable host media. Due to their safety function, the behaviour of the Excavation Damaged Zone (EDZ) that develops around galleries during their drilling can affect the safety of repository facilities (Armand et al. 2014). In fact, the underground excavation process induces rock damage and the development of an EDZ dominated by fracturing process. Understanding and predicting the latter are of paramount importance. Among the different envisaged media, the Callovo-Oxfordian (COx) claystone is studied in France (Andra 2005). It is an indurated sedimentary clay rock which has a complex microstructure exhibiting multi-scale heterogeneities. At meso-scale (i.e. mineral inclusion scale), the COx claystone is composed of several types of minerals with scattered mineralogical characteristics. It is well known that large-scale phenomena (deformation, failure, etc.) take their origin from small-scale processes, as at mineral inclusions and clay matrix scales for clay rocks. Questions have risen on how micro- and meso-structural characteristics of heterogeneous rocks can enrich the macroscale constitutive behaviour to predict deformation and failure processes. Consequently, the numerical modelling of the mechanical behaviour of the clay rock is realised by considering its micro- and meso-structural characteristics. The behaviour of the COx claystone and its damage under mechanical solicitations are modelled at several scales. Firstly, an insight of micro-damage and meso-cracking is obtained by small-scale modelling. Then, macroscale shear failure is reproduced at the scale of laboratory samples. Finally, the macroscale behaviour of the EDZ is studied with the development of shear bands in relation to the failure types at mesoscale and to the damage at microscale.

2 CALLOVO-OXFORDIAN CLAY ROCK STRUCTURE

The heterogeneous clay rock microstructure is composed of several mineral types: tectosilicates (quartz, ~18%), carbonates (calcite, ~30%), heavy minerals (pyrite, ~2%), and clay minerals (~50%) in large proportion in the clay-rich zone of the rock (Andra 2005; Armand et al. 2014; Robinet at al. 2012). Quartz and carbonate mineral inclusions are embedded in a clay matrix and the size of a representative mesostructure of the claystone is of 100×100×100 µm³ (Cosenza et al. 2015; Robinet et al. 2012). The spatial distribution and the morphology of the mineral inclusions are considered (Pardoen et al. 2020). Realistic mesostructures are numerically modelled by 2D periodic Representative Elementary Areas (REA) with the different mineral phases and their spatial arrangement (Figure 1). The generation algorithm uses a Voronoï tessellation in which the cells represent mineral inclusions and large clay aggregates (Pardoen et al. 2020). Furthermore, experimental evidences have shown that potential decohesion mechanisms develop around mineral inclusions and micro-cracks propagate within the clay matrix (Desbois et al. 2017). Therefore, the damage between the minerals are considered (van den Eijnden et al. 2016; Pardoen et al. 2020).

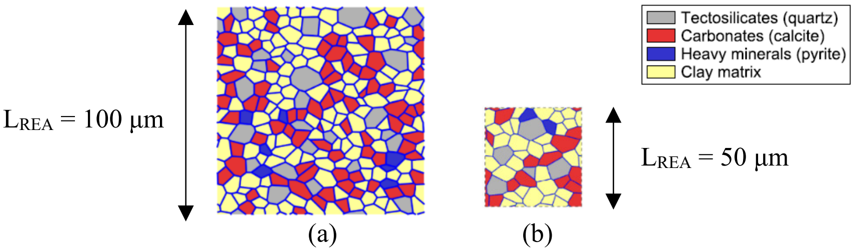

Figure 1. Schematic representation of representative numerical mesostructures of a heterogeneous rock of dimensions: (a) 100 µm and (b) 50 µm.

3 DOUBLE-SCALE MODEL

A double-scale FEM×FEM numerical approach is used with finite element computations at both scales (van den Eijnden et al. 2016). The macroscale constitutive behaviour, in the macroscale computation, is derived from the overall mesoscale response of 2D periodic REA, by mesoscale computation. The scale transition (downscaling macro to meso) is realised by enforcing periodic boundary conditions on the mesoscale model (REA) which results in the macrostrain tensor ε_{ij}^{M}:

$$du_i^{m,S} = \varepsilon_{ij}^{M}\, y_j = \varepsilon_{ij}^{M}\, dx_j^{m,S} \tag{1}$$

where $x_i^{m,S}$, $u_i^{m,S}$, and y_i are the mesoscale boundary positions, displacements, and periodic vectors.

The mesoscale model reproduces the clay rock behaviour, including the deformation and damage processes. The generated REAs (Figure 1) are defined as assemblies of (isotropic linear) elastic deformable continuous solid minerals in interaction with cohesive crack models. The latter are damageable cohesive interfaces which permit material softening due to deformation and movements.

The cohesive laws in tangential and normal contact directions are defined independently by:

$$c_{n/t} = \frac{1 - D_{n/t}}{D_{n/t}} \frac{\Delta u_{n/t}}{\delta_{n/t}^{c}} c_{n/t}^{max} \tag{2}$$

where *n* and *t* subscripts correspond to normal and tangential directions, $c_{n/t}$ are interface cohesion forces, $c_{n/t}^{max}$ are maximal cohesion forces, $\Delta u_{n/t}$ are interface relative displacements. Then, $D_{n/t}$ are softening parameters representing the interface degradation state $D_{n/t}^{0} \leq D_{n/t} \leq 1$, $\delta_{n/t}^{c}$ are critical relative displacements inducing complete decohesion ($D_{n/t} = 1$, $c_{n/t} = 0$), and solid interpenetration is not allowed ($\Delta u_n \geq 0$). Following the above definitions, numerous possible mesocrack paths can develop in the mesostructure.

The multiscale method allows a scale transition from the mesoscopic scale to the macroscale (upscaling meso to macro). From the mesoscale, a homogenised response is derived and used as an implicit constitutive law at macroscale, by computational homogenisation (Kouznetsova et al. 2001). The homogenised total stress tensor σ_{ij}^{M}, i.e. the mesoscopic stress average over the REA, is:

$$\sigma_{ij}^{M} = \frac{1}{V} \int_{S} t_i \, y_j \, dS \tag{3}$$

where V, S, and t_i are the mesostructure volume, outer surface, and boundary traction surface forces.

Concerning the macroscale model, the modelling of the fracturing process is realised with strain localisation in shear bands. The latter are considered as a precursor to shear fractures in quasi-brittle geomaterials. A model properly reproducing the strain localisation with FEM is used. It is the coupled local second gradient model which involves a regularisation method (Pardoen et al. 2015).

4 SHEAR FAILURE FROM MESO- TO MACRO- SCALES

The shear failure of the clay rock across scales is modelled hereafter. It is predicted from mesocracking, within the clay matrix and between mineral inclusions, to large-scale fractures, as observed on laboratory rock samples and around underground galleries (section 5). At microscale, the mechanical parameters used in the modelling are detailed in Table 1 (Pardoen et al. 2020).

Table 1. Microscale mechanical parameters.

Minerals	E [GPa]	ν [-]	Area fraction [%]	
Tectosilicates (quartz)	95	0.074	18	
Carbonates (calcite)	84	0.317	30	
Heavy minerals (pyrite)	305	0.154	2	
Clay matrix	2.3	0.110	50	
Interfaces	$\delta_{t/n}^{c}$ [-]	$D_{t/n}^{0}$ [-]	c_t^{max} [MPa]	c_n^{max} [MPa]
	0.1	0.001	2.5	1.0

At mesoscale, the REA is subjected to biaxial compression under constant confining pressure σ_{11}^{M} = 12 MPa and increasing deviatoric vertical load $q^M = \sigma_{22}^{M} - \sigma_{11}^{M}$, by vertical strain ε_{22}^{M} increase. The crack pattern in one REA, at different vertical strains ε_{22}^{M}, is depicted in Figure 2 (a-c) by the mineral contacts in softening and in complete decohesion. Under this type of loading, the decohesion appears in a localised manner (Pardoen et al. 2020). After the development of damage at the mineral contacts, a full mesoscale crack propagates through the entire REA and leads to material softening (Pardoen et al. 2020). The mesoscale homogenised mechanical response curve, i.e. deviatoric stress versus vertical strain $q^M - \varepsilon_{22}^{M}$, is shown in Figure 3 (e). A softening response, i.e. decrease of q^M under ε_{22}^{M} increase, is well modelled for quasi-brittle rock. The homogenised shear strain ε_{12}^{M} of the REA, during the biaxial compression loading test, is illustrated in Figure 2 (d). Mourlas et al. (2023) show that the orientation of the REA mesocracking and the sign of the homogenised shear strain ε_{12}^{M} can indicate the orientation of the shear band in macroscale. In this case, $\varepsilon_{12}^{M} > 0$ indicates that the macro strain localisation will most probably develop in the same direction as the mesocracking of the REA.

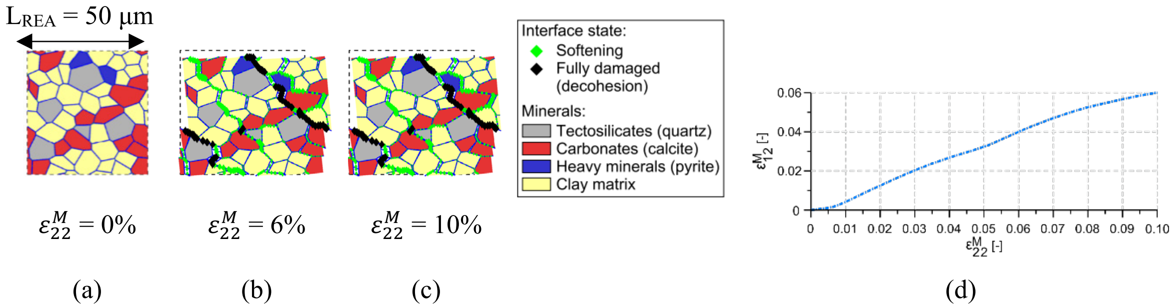

Figure 2. Mesocrack development in rock mesostructure: (a) initial mesostructure, (b-c) damage under increasing deviatoric vertical loading, and (d) homogenised shear strain evolution.

At the scale of rock laboratory samples (few centimetres of dimension), the biaxial compression test is performed with double-scale modelling approach. The results are illustrated in Figure 3. The shear bands are represented as localisation of Von Mises' equivalent deviatoric total strain $\hat{\varepsilon}_{eq} = \sqrt{\frac{2}{3}\hat{\varepsilon}_{ij}\hat{\varepsilon}_{ij}}$, with the deviatoric strain tensor $\hat{\varepsilon}_{ij} = \varepsilon_{ij} - \frac{\varepsilon_{kk}}{3}\delta_{ij}$. The strain is not homogeneous in the sample and concentrates inside a shear band. The results of both macroscale (double-scale) and mesoscale analyses, in terms of stress-strain $q - \varepsilon_{22}$ curves are illustrated in Figure 3 (e). The development of a shear band through the clay rock specimen engenders a softening material behaviour.

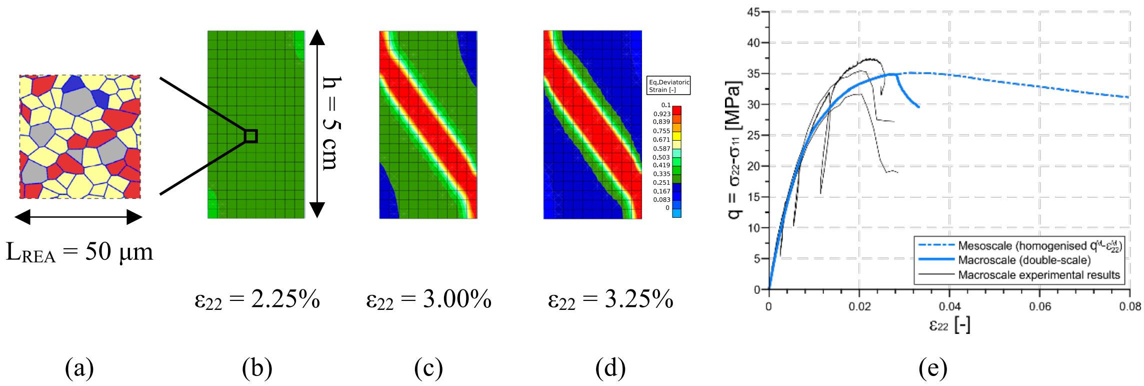

Figure 3. Shear band development in rock sample: (a) initial mesostructure, (b-d) strain localisation under increasing deviatoric vertical loading, and (e) mesoscale and macroscale stress–strain response curves.

The deformation of the material mesostructure, inside and outside the macro shear band, is presented in Figure 4. Outside, the mesostructure is not deformed neither damaged; while inside, it is significantly deformed and damaged. The results show that the orientation of the shear band at macroscale corresponds with the crack orientation in the mesoscale (Figure 2).

5 EXCAVATION DAMAGED ZONE MODELLING

An excavation of an unsupported gallery in the COx claystone is performed in 2D plane strain state. The objective is to show the effect of the mesoscale clay rock behaviour on the macroscale EDZ development, modelled by shear bands. The gallery is parallel to the minor horizontal principal total stress σ_h = 12.4 MPa and the initial stress state in the gallery section is anisotropic with σ_v = 12.7 MPa and σ_H = 1.3 σ_h = 16.12 MPa in the vertical and horizontal directions. The stress reduction at gallery wall is defined by $\sigma_{H/v,wall} = (1 - \lambda)\sigma_{H/v,0}$ with the deconfinement rate λ = 0→1. The Figure 5 depicts the development of the shear bands around the gallery during and at the end of the

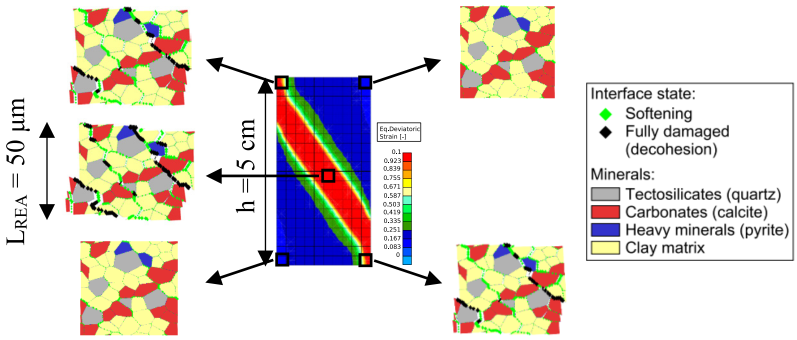

Figure 4. Shear band in rock sample at vertical strain ε_{22} = 3.25 % and deformed mesostructures.

excavation. The shear bands develop close to the end of the excavation preferentially above the gallery, due to anisotropic stress, in the direction of the minor principal stress in the gallery section.

The link between mesocracking (i.e. mesoscale failure of the REA) and macro shear banding (i.e. macroscale shear failure in the EDZ) is studied. Figure 6 illustrates the large-scale shear band pattern around the gallery, at the end of excavation, and the small-scale deformed and damaged mesostructures. The latter are shown in different locations inside and outside the macro strain localisation zones. In the macro shear bands, the mesostructures are deformed and damaged and show different mesocrack patterns, either with horizontal or diagonal mesocrack (Mourlas et al. 2023). Depending on the location around the gallery, the damage at microscale can either be in shearing or in opening mode. The modelled EDZ presents mixed-mode fractures (shear-opening) close to the gallery wall, as observed in the EDZ (Armand et al. 2014). The measured size of the mixed fracture zone is displayed in Figure 6 (dashed line) with a good agreement of the numerical results.

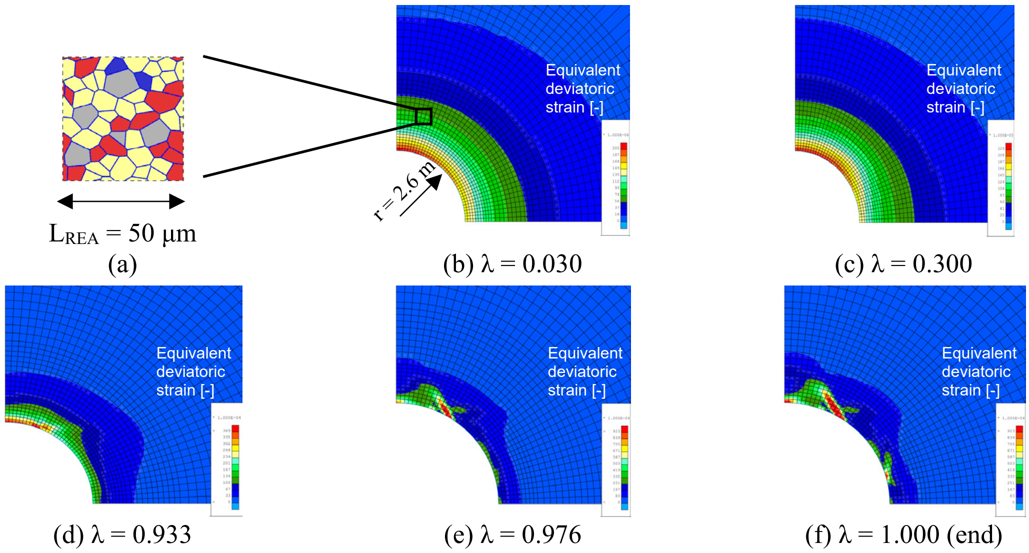

Figure 5. Shear band development in rock around gallery: (a) initial mesostructure, (b-e) strain localisation during the excavation, and (f) at the end of excavation.

6 CONCLUSION

The proposed approach highlights the multi-scale aspects to consider to reproduce the mechanical behaviour of the excavation fractured zone in clay rock. The focus is on the numerical modelling from microscopic to macroscopic behaviours of damaged rock. At the scale of mineral inclusions and clay matrix, the mesoscale model allows to reproduce the micro-damage and meso-cracking while considering the morphology and heterogeneity of minerals. At the scale of laboratory samples, the double-scale model allows to reproduce shear failure by shear banding. The results indicate that

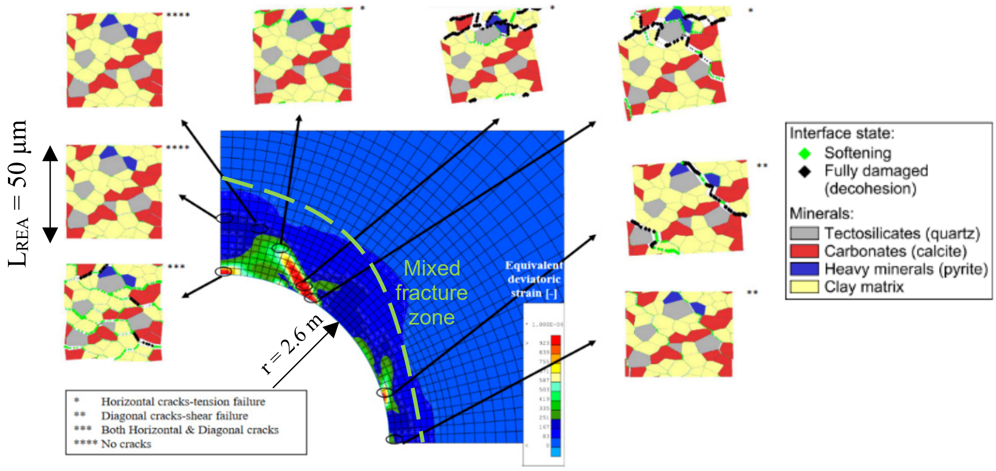

Figure 6. Shear band pattern in rock around gallery at the end of excavation and deformed mesostructures.

the model can capture the shear failure and the material response measured in laboratory biaxial compression tests. At the scale of underground structures, the double-scale model reproduces the development of the excavation fractured zone around galleries. The modelling shows the relation between deformations, damages, and failures across scales in heterogeneous rocks (Mourlas et al. 2023). It demonstrates that the macroscale rock behaviour and failure depend on its meso- and micro-structural behaviours, including potential mesoscale crack formations from microscale damage mechanisms. The results highlight the possibilities to consider micro- and meso-structural characteristics in the modelling of rock damaged zone related to engineering applications.

REFERENCES

Andra 2005. Dossier. 2005 Argile. Synthesis: Evaluation of the feasibility of a geological repository in an argillaceous formation, Meuse/Haute Marne site. *Technical report*, Paris, France.

Armand, G., Leveau, F., Nussbaum, C., de La Vaissiere, R., Noiret, A., Jaeggi, D., Landrein, P., and Righini, C. 2014. Geometry and properties of the excavation-induced fractures at the Meuse/Haute-Marne URL drifts. *Rock Mechanics and Rock Engineering*, 47(1), pp. 21–41.

Cosenza, P., Prêt, D., Giraud, A., and Hedan, S. 2015. Effect of the local clay distribution on the effective elastic properties of shales. *Mechanics of Materials*, 84, pp. 55–74.

Desbois, G., Höhne, N., Urai, J.-L., Bésuelle, P., and Viggiani, G. 2017. Deformation in cemented mudrock (Callovo-Oxfordian Clay) by microcracking, granular flow and phyllosilicate plasticity: insights from triaxial deformation, broad ion beam polishing and scanning electron microscopy.*Solid Earth*,8,pp.291-305

Kouznetsova, V., Brekelmans, A. M., and Baaijens, P. T. 2001. An approach to micro-macro modeling of heterogeneous materials. *Computational Mechanics volume*, 27(1), pp. 37–48.

Mourlas, C., Pardoen, B., and Bésuelle, P. 2023. Large-scale failure prediction of clay rock from small-scale damage mechanisms of the rock medium using multiscale modelling. *International Journal for Numerical and Analytical Methods in Geomechanics*. 47, pp. 1254–1288.

Pardoen, B., Seyedi, D. M., and Collin, F. 2015. Shear banding modelling in cross-anisotropic rocks. *International Journal of Solids and Structures*, 72, pp. 63–87.

Pardoen, B., Bésuelle, P., Dal Pont, S., Cosenza, P., and Desrues, J. 2020. Accounting for Small-Scale Heterogeneity and Variability of Clay Rock in Homogenised Numerical Micromechanical Response and Microcracking. *Rock Mechanics and Rock Engineering*, 53(6), pp. 2727–46.

Robinet, J.-C., Sardini, P., Coelho, D., Parneix, J.-C., Prêt, D., Sammartino, S., Boller, E., and Altmann, S. 2012. Effects of mineral distribution at mesoscopic scale on solute diffusion in a clay-rich rock: Example of the Callovo–Oxfordian mudstone (Bure, France). *Water Resources Research*, 48(5). W05554.

van den Eijnden, A., Bésuelle, P., Chambon, R., and Collin, F. 2016. A FE^2 modelling approach to hydromechanical coupling in cracking-induced localization problems. *International Journal of Solids and Structures.*, 97–98, pp.475–488.