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A numerical study of effective mechanical behaviors of rock like materials based on Fast Fourier Transform

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ABSTRACT

This paper is devoted to the numerical modeling of effective mechanical behaviors of rock like materials by taking into account effects of micro-structure. The numerical model will be based on the Fast Fourier Transform (FFT) technique. We consider a class of rock materials with a microstructure which can be represented by a continuous matrix phase in which are embedded mineral inclusions. One or several constituent phases exhibit a nonlinear inelastic behavior. The proposed numerical model is firstly assessed by comparing numerical results with reference solutions obtained by direct finite element simulations. It will be then applied to a typical clayey rock which is constituted by an elastic–plastic clay matrix which is reinforced by linear elastic quartz and calcite grains. The proposed numerical model is further extended by including the progressive damage process due to the growth of micro-cracks. Comparisons between numerical results and experimental data will be presented to assess the efficiency of the numerical model.

1. Introduction

During the last decades, clayey rocks have been largely investigated in many countries as a potential geological barrier for underground radioactive waste disposal and sequestration of residual gas. Clayey rocks also constitute the cap rock of many oil and gas reservoirs. On the other hand, shales are investigated as reservoir rocks for the optimal exploration of shale gas. In all these applications, it is crucial to characterize and describe both short and long term hydromechanical behaviors of clayey rocks, in particular plastic deformation and damage process, as well as permeability evolution. As a representative clayey rock, we consider here the Callovo–Oxfordian (COX) claystone from the underground research laboratory of Andra, the French National Agency for radioactive waste management. Extensive laboratory studies have been conducted this material and we do not intend to give here an exhaustive review of all obtained results (Andra, 2005; 2012). Basically, the inelastic mechanical behaviors of the COX claystone can be characterized by the plastic deformation and microcrack induced damage in the clay matrix and at interfaces. The macroscopic responses are strongly influenced by its mineral compositions and the water saturation degree due to the presence of swelling clay minerals such as smectite. Time-dependent behaviours have also been investigated thorough creep tests and as a first approximation can be attributed to viscoplastic deformation and subcritical propagation of microcracks of the clay matrix. Based on experimental results, different kinds of macroscopic constitutive models have first been proposed to describe the elastic, plastic, viscoplastic and damage behaviors of the COX claystone, for instance Chiarelli et al. (2003); Shao et al. (2006); Hoxha et al. (2007). These macroscopic models can generally capture the overall responses of the

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material but fail to properly taking into account effects of micro-structure. For example, the macroscopic models are not able to explicitly describe the effects of mineral compositions and spatial distribution of mineral inclusions. In order to improve and complete the macroscopic models, an important effort has been made during the last years on the development of micro-mechanical models based on various homogenization techniques. Concerning clayey rocks, several micro-macro models have also been proposed, for instance Abou-Chakra Guéry et al. (2008); Shen et al. (2012b); 2013). In these models, the claystone has been represented as a three phase composite constituted by a clay matrix and quartz and calcite grains. The clay matrix has been further considered as a porous medium composed of a solid phase and spherical pores (Shen et al., 2012b, 2013). Some other models have been proposed for modeling the time-dependent behaviours of the claystone (Huang and Shao, 2013; Huang et al., 2014, 2015; Bikong et al., 2015). The models provide an interesting alternative way for modeling heterogeneous rock like materials taking into account effects of micro-structures. However, in order to obtain analytical or semi-analytical formulations, strong assumptions were generally introduced on the description of microstructure. For instance, all mineral inclusions and pores were assumed to be of spherical form and randomly embedded in the solid phase. The real microstructure of most rock like materials is obviously more complex than this simplified representation. In view of not only validating analytical micro-mechanical models but also studying effects of microstructure on macroscopic behaviors, it is needed to develop numerical simulations based a realistic description which should be as close as possible to the real microstructure.

For this purpose, we propose here to apply a numerical method based on the Fast Fourier Transform (FFT). This mathematical technique was successfully applied by Moulinec and Suquet (1994, 1998) as an alternative approach of the finite element method to compute the effective properties of composite materials with a periodic microstructure. This approach was further improved by an accelerated scheme to improve its computational efficiency (Eyre and Milton, 1999; Michel et al., 1999, 2000) and to extend its ability to voids and rigid inclusions (Michel et al., 2001). Furthermore, Monchiet et Bonnet (Monchiet and Bonnet, 2012) have proposed a polarization-based FFT iterative scheme for computing the effective properties of elastic composites with arbitrary contrast and containing imperfect interfaces. Brisard and Dormieux (Brisard and Dormieux, 2010, 2012) have proposed a general variational framework for FFT-based methods and to combine Galerkin approximation techniques with the principle of Hashin and Shtrikman to derive a new FFT-based numerical scheme for the homogenization of linear composites. Based on such framework, FFT-based methods have been applied to homogenization of permeability of porous materials (Bignonnet and Dormieux, 2014). Some recent works have been devoted to homogenization of elastic layered composites with interfaces oscillating using a FFT-based method (LeQuang et al., 2014). Multi-scale approaches using fast Fourier transforms have been proposed for modeling progressive damage of composite materials (Spahn et al., 2014) and for modeling viscoplastic behaviors of two-phase materials (Lee et al., 2011) and polycrystal materials (Lebensohn et al., 2012). Some applications of FFT based micro-mechanical modeling to nonlinear behaviors of rock-like materials have also been presented (Jiang and Shao, 2012). The main advantage of FFT-based approaches is ability to efficiently consider non-regular geometrical forms of microstructure due to the fact that no volumetric meshing is needed since the heterogeneous material field is discretized into a series of grid points. Different mechanical properties can be assigned on each point according to its location inside the heterogeneous micro-structure. The overall responses at the macroscopic scale are then obtained by the volumetric average on the unit cell of the local stress and strain fields at the microscopic scale (Hill, 1963; Li and Wang, 2008). In this work, based on the FFT technique and the previous work by Jiang and Shao (2012), a numerical micro-mechanical model will be proposed to describe the inelastic behavior of the COX claystone. To this end, the clay matrix will described by an elastic plastic model based on a pressure sensitive yield criterion. Then, in order to describe the material softening behavior due to induced damage process, an elastic damage model will be introduced for the calcite grains. Some sensitivity studies will also be presented to show effects of different micro-structures on macroscopic responses. The efficiency of the proposed numerical model will be firstly verified against reference solutions obtained by direct finite element simulations and through comparisons between numerical results and experimental data.

2. Microstructure of COX claystone

The claystone studied here is from the underground research laboratory constructed by Andra in the North-East region of France. The main facilities of the laboratory are located at the depth from 445m to 490m and excavated in a 200m thick sub-horizontal layer of Callovo-Oxfordian formation. The COX claystone is characterized by its low permeability and relatively high mechanical strength. The mineralogical compositions vary with the depth and contain three main phases: clay matrix, calcite grains and tectosilicates mainly composed of quartz grains. A representative microstructure picture of the COX claystone is shown in Fig. 1 (Robinet, 2008). At the depth corresponding to the underground research laboratory, the average mineralogical compositions are 40 to 50% of clay minerals, 20 to 27% of calcite and 23 à 25% of quartz. There is also a small quantity of other minerals such pyrite, mica, dolomite, halite and gypse.

The microstructure of the COX claystone is heterogeneous at different scales. In view of micro-macro modeling of its mechanical behaviors, it seems that the following relevant scales should be considered:

- At the nanometer and micrometer scales ($\sim\mu$m), the clay minerals have a complex organization with several scales (sheets, particles, aggregates). The size of pores varies from nanometer to micrometer and respectively associated with intra-particular voids (between clay sheets) and inter-particular voids (between particles). It was found that the porosity of the COX claystone contains two representative average sizes, 4 nm and 20 nm respectively (Andra, 2005); Robinet (2008). The total porosity can also vary with the depth.