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A micromechanical model for porous materials with a reinforced matrix

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ABSTRACT

In this study a micromechanical model is proposed for ductile porous material whose matrix is reinforced by small inclusions. The solid phase is described by a pressure sensitive plastic model. Based on works of Maghous et al. [6], a macroscopic plastic criterion is firstly obtained by using a two-step homogenization procedure. The effect of porosity at the mesoscale and the influence of inclusions at the microscale are taken into account simultaneously by this criterion. With a non-associated plastic flow rule, the micro-macro model is applied to modeling of mechanical behavior of a cement paste. In particular, we have considered at the microscopic scale the formation of calcite grains by carbonation process in the solid matrix. The studied cement paste is then seen as a reinforced matrix–pore system. Comparisons between numerical results and experimental data show that the proposed model is able to capture the main features of the mechanical behavior of the studied material.

1. Introduction

The microstructure of composites has a great effect on the macroscopic mechanical behavior. For example, the pores or inclusions significantly affect the mechanical strength and deformation behavior of the heterogeneous material. Recently, in the context of geological disposal of radioactive wastes, various clayey rocks have been investigated as a possible geological barrier. It was found that the macroscopic mechanical behaviors of these rocks strongly depend on the mineralogical compositions and microstructure evolutions. The mineralogical analysis has revealed that at the mesoscopic scale, this class of clayey rocks is composed of a porous clay matrix which is reinforced by mineral inclusions essentially composed of quartz and calcite grains. The size of pores is much smaller than the one of grains. Various micromechanical models have been proposed to describe the elastoplastic behaviors of clayey rocks ([1,11,12], etc.). The studied rock has been schematized as a porous matrix reinforced by inclusions at the mesoscale. Recently, the strength properties of this class of composite material (microporous matrix – inclusions) have also been studied by He et al. [4] (see also [5]) with two step homogenization. The elliptic criterion of Maghous et al. [6] is adopted to describe the mechanical behaviors of microporous medium at the microscale. In the second homogenization procedure, the limit analysis theory is used to capture the influence of inclusions. But for some others rocks, cement-based materials or polymers, the pore size can be much bigger than that of inclusions. For example, new small calcite grains will be generated in the cement paste due to the carbonation process. The solid matrix will be reinforced by these small calcite ($CaCO_3$) grains at the microscopic scale. This type of material can be seen as a porous material with a reinforced matrix whose solid phase is described by a pressure-dependent plastic model (Fig. 1). The objective of this paper is to extend the works of Maghous et al. [6] and establish a micro-macro model for this class of composite materials by using a two-step nonlinear homogenization technique. Based on the results of Maghous et al. [6], the variational homogenization methods will be used twice to obtain the macroscopic criterion for a porous medium with a reinforced matrix by small rigid inclusions at the microscopic scale.

The paper is organized as follows. In Section 2, a micromechanical constitutive model will be firstly formulated for the studied porous materials with a reinforced and compressible matrix. The effect of porosity is taken into account at the mesoscale and the influence of inclusions is considered at the microscale. Then the model is completed by a macroscopic plastic potential and a plastic hardening law. In Section 3, the proposed non-associated model is implemented and applied to describe the macroscopic mechanical behavior of a cement-based material considering the carbonation effects.

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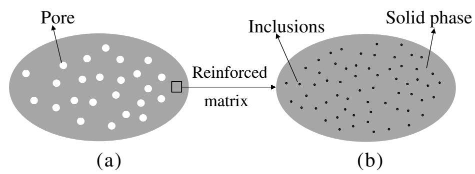

Fig. 1. Porous material with a reinforced matrix.

2. Macroscopic criterion of porous media with a reinforced matrix

In this section, we aim at determining the macroscopic plastic criterion of the porous medium with a reinforced matrix (Fig. 1). The solid phase is compressible and obeys to a Drucker–Prager criterion. Comparing with the solid phase, the inclusion are assumed rigid, spherical and randomly distributed in the matrix. To consider the effects of pores and inclusion simultaneously, a two-step homogenization procedure will be adopted to formulate the macroscopic plastic criterion of the studied composite (*microscale to mesoscale, mesoscale to macroscale*).

As illustrated in Fig. 1, the volume fraction ρ of inclusions at the microscale and the porosity f of the porous medium are given by:

$$\rho = \frac{\Omega_i}{\Omega_i + \Omega_s}, \quad f = \frac{\Omega_p}{\Omega_i + \Omega_s + \Omega_p} \tag{1}$$

where Ω_i, Ω_s and Ω_p are volumes of inclusions, solid phase in the matrix and the pore of the composite, respectively.

2.1. Homogenization from micro to meso for the effect of inclusions

In this transition from microscale to mesoscale, the solid phase of the reinforced matrix is assumed to obey to a Drucker–Prager criterion:

$$\phi^s(\boldsymbol{\sigma}) = \sigma_d + T(\sigma_m - h) \le 0 \tag{2}$$

where $\boldsymbol{\sigma}$ denotes the local stress in the solid phase at the microscale, $\sigma_m = \mathrm{tr}\boldsymbol{\sigma}/3$ the mean stress, and $\sigma_d = \sqrt{\boldsymbol{\sigma}' : \boldsymbol{\sigma}'}$ the equivalent stress (with $\boldsymbol{\sigma}' = \boldsymbol{\sigma} - \sigma_m \boldsymbol{1}$). The parameter h represents the hydrostatic tensile strength while T denotes the frictional coefficient.

For geomaterials, the plastic potential of the solid phase is given by:

$$g^s(\boldsymbol{\sigma}) = \sigma_d + t\sigma_m \tag{3}$$

the parameter t defines the dilatancy coefficient which controls the volumetric plastic strain.

For a solid phase reinforced by rigid inclusions, we take advantage of results obtained by Maghous et al. [6] who made use of a non linear homogenization technique based on the so-called modified secant method. Note that this method was originally proposed by Ponte Castaneda [8,9] as a variational method and was later interpreted as "a modified secant method" by [10,13,14]. These authors obtained a criterion and a flow rule for a matrix (Drucker–Prager type) reinforced by rigid inclusions.

Here we recall the main steps of the modified secant method using in [6]. With (2) and (3), the support function π^s can be calculated with the help of a sequence of potentials ψ_a using the technique proposed in [2]. Then the stress state is defined by means of a potential ψ_a and an isotropic prestress σ_0^p: $\boldsymbol{\sigma} = \partial\psi_a/\partial \boldsymbol{d} + \sigma_0^p \boldsymbol{1}$, which can be rewritten with the secant bulk and shear moduli and the isotropic prestress in the following form:

$$\boldsymbol{\sigma} = 2\mu^s \boldsymbol{d}' + \kappa^s d_v \boldsymbol{1} + \sigma^p \boldsymbol{1} \tag{4}$$

where μ^s, κ^s and σ^p are functions of plastic deformation $\boldsymbol{d}(d_v, d_d)$[1] which is non-uniform in the solid phase. For the simplicity, an effective strain rate $\boldsymbol{d}^e$ (average of $\boldsymbol{d}$ over the matrix) is introduced. Then these three non-uniform moduli can be expressed in term of $\boldsymbol{d}^e$ ($\mu^s(\boldsymbol{d}) = \mu^s_{eq}$, $\kappa^s(\boldsymbol{d}) = \kappa^s_{eq}$ and $\sigma^p(\boldsymbol{d}) = \sigma^p_{eq}$). The homogenized behavior takes the form:

$$\begin{aligned} &\tilde{\boldsymbol{\sigma}} = \mathbb{C}^{hom} : \boldsymbol{D} + \tilde{\sigma}^p \boldsymbol{1}; \\ &\mathbb{C}^{hom}(d_v^e, d_d^e) = 3\kappa^{hom}(\kappa^s_{eq}, \mu^s_{eq})\mathbb{J} + 2\mu^{hom}(\kappa^s_{eq}, \mu^s_{eq})\mathbb{K} \end{aligned} \tag{5}$$

The symbol "∼" is used here in order to make difference between the mesoscopic stress field $\tilde{\boldsymbol{\sigma}}$ and the microscopic one in the solid phase $\boldsymbol{\sigma}$. $\boldsymbol{\Sigma}$ is used to denote the macroscopic stress of the composite.

Owing to the assumption of rigid inclusions, the macroscopic prestress simply reads $\tilde{\sigma}^p = \sigma^p_{eq}$. The state equations are expressed as:

$$\tilde{\sigma}_m = \kappa^{hom} D_v + \tilde{\sigma}^p; \qquad \tilde{\sigma}_d = 2\mu^{hom} D_d \tag{6}$$

Following [2], the relation between the effective strain rates in the solid phase and the loading $\boldsymbol{D}$ is:

$$\begin{aligned} &\frac{1}{2}(1-\rho){d_v^e}^2 = \frac{1}{2}\frac{\partial \kappa^{hom}}{\partial \kappa^s_{eq}} D_v^2 + \frac{\partial \mu^{hom}}{\partial \kappa^s_{eq}} D_d^2 \\ &(1-\rho){d_d^e}^2 = \frac{1}{2}\frac{\partial \kappa^{hom}}{\partial \mu^s_{eq}} D_v^2 + \frac{\partial \mu^{hom}}{\partial \mu^s_{eq}} D_d^2 \end{aligned} \tag{7}$$

The homogenized secant moduli κ^{hom} and μ^{hom} are evaluated with the help of the Mori–Tanaka scheme which coincides here (case of rigid inclusions) with the Hashin-Shtrikman lower bound:

$$\kappa^{hom} = \frac{3\kappa^s_{eq} + 4\rho\mu^s_{eq}}{3(1-\rho)}, \quad \mu^{hom} = \mu^s_{eq}\frac{\kappa^s_{eq}(6+9\rho) + \mu^s_{eq}(12+8\rho)}{6(1-\rho)(\kappa^s_{eq} + 2\mu^s_{eq})} \tag{8}$$

The strength criterion and the plastic potential of the solid phase reinforced by rigid inclusions (Fig. 1b) take the following form:

$$\begin{aligned} &\phi^m = \widetilde{\sigma}_d + \widetilde{T}(\widetilde{\sigma}_m - h) \le 0; \quad \widetilde{T} = T\sqrt{1+\frac{3}{2}\rho}\ \frac{\sqrt{1-\frac{2}{3}\rho t^2}}{1-\frac{2}{3}\rho t T} \\ &g^m = \widetilde{\sigma}_d + \widetilde{t}\widetilde{\sigma}_m; \quad \widetilde{t} = t\sqrt{\frac{1+\frac{3}{2}\rho}{1-\frac{2}{3}\rho t^2}} \end{aligned} \tag{9}$$

2.2. Homogenization from meso to macro for the effect of pores

In the second homogenization, the effect of pores in the porous medium will be considered (Fig. 1a). The reinforced matrix is described by (9). Comparing the equations (9) with (2) and (3), the same forms are found for the criterion and the plastic potential. The non-linear homogenization technique proposed by Maghous et al. [6] for the porous medium will be adopted here.

Different with the case of solid phase reinforced by rigid inclusion, the macroscopic prestress changes to $\Sigma^p = \frac{\kappa^{hom}}{\kappa^{em}_{eq}}\tilde{\sigma}^p_{eq}$, the state equation (6) becomes:

$$\Sigma_m = \kappa^{hom}\left(D_v + \frac{\tilde{\sigma}^p_{eq}}{\kappa^{em}_{eq}}\right); \qquad \Sigma_d = 2\mu^{hom} D_d \tag{10}$$

[1] Where $d_v = \mathrm{tr}\boldsymbol{d}$, $d_d = \sqrt{\boldsymbol{d}' : \boldsymbol{d}'}$ with $\boldsymbol{d}' = \boldsymbol{d} - \frac{d_v}{3}\boldsymbol{1}$.