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Plastic-damage modeling of saturated quasi-brittle shales

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ABSTRACT

The constitutive modeling of shales is an important topic in the geomechanics community as it is often encountered in advanced applications such as nuclear waste storage, CO2 sequestration, and unconventional oil and gas exploitation. The goal of this work is to describe, within a unique plastic-damage framework, the full mechanical behavior of shales such as pre-peak hardening plasticity, non-linearity in the onset of inelastic strains, dilatancy, post-peak softening, and degradation of the elastic parameters. The model validation against three sets of triaxial experimental results on shale demonstrates its capability to reproduce the main mechanical characteristics.

1. Introduction

Shale is a clay rich material usually identified by the feature of having more than 35% clay mineral content with bonding between the clay particles that can be stronger or weaker depending on mineralogy.¹ Because of deposition and sedimentation processes, many shales have a layered structure in which the clay particles are oriented, conferring initial orthotropic properties to the material. Given this broad classification, common features of the constitutive behavior of shales are not always clearly identifiable. From a mechanical point of view, the rheological base of shale was thoroughly discussed in the work of Parisio et al. (2015),² i.e., the behavior of shale is assumed to belong to the class of quasi-brittle geomaterials. In quasi-brittle materials the accumulation of plastic strains during the inelastic phase prior to cracking is small compared to the total strains after failure.³ While the clay rich matrix confers plasticity properties to the materials, the bonding breakage during loading can be associated with damageable-like behavior. Experimental results on Opalinus Clay,^{4–8} LaBiche Shale,⁹ Tournemire Shale,^{10,11} Callovo-Oxfordian Shale,¹² North Sea Shale¹³ and Dotternhausen shale¹⁴ show that: (1) the complete deformation process in conventional triaxial compression tests can be summed up as an initial phase of linear elastic deformation with no dissipation, followed by the accumulation of small permanent strains originated by microcracking and bonding breakage (same order of magnitude as the elastic ones) until the peak of stress is reached; (2) peak conditions are followed by a softening phase, in which the breaking of brittle bonding accumulates, permanent strain becomes significant, the material is dilating and a reduction of elasticity is usually observed until a final residual deviatoric stress plateau is reached. A comparison of deformation and strength characteristics of different shales can be found in Vilarrasa et al. (2013).¹⁵ At high levels of confinement stress, a transition into cataclastic compressive deformation was shown in Rybacki et al. (2015).¹⁴ Although this feature has been widely investigated in other sedimentary geomaterials like sandstones¹⁷ and limestones,^{17–19} in shale only few and limited data exist.¹ In undrained conditions, the shear phase is performed by not allowing water to migrate out of the sample. This generates an increase in the pore water pressure.¹³ The magnitude of the pore water pressure increase depends on the poromechanical properties, i.e., solid and water compressibility, as well as on the volumetric strain behavior. Dilatancy in the inelastic phase generates volumetric expansion, i.e., additional pore space. The result is a decrease in pore water pressure in the sample.

Given these peculiar features, shale in particular and quasi-brittle geomaterials in general have been often modeled with coupled damageplasticity constitutive models.^{20–30,51} The plastic part is usually responsible for the permanent inelastic strain accumulation, while damage confers the brittleness to the material, i.e., softening and degradation of elastic moduli. Given the layered structure of the material, many shales exhibit anisotropic deformation and strength properties.^{7,10,11,31,32} This subject is beyond the scope of the present work, and it will be presented and developed in detail in a separate paper that is in preparation.

The main goal of the present work is the development and validation of a plastic-damage constitutive model in an isotropic framework. The proposed model is a direct extension of the previous

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constitutive model that was developed in the work of Parisio et al. (2015),² where plasticity was formulated in the effective stress space.^{33–35} Details on the advantages of a model that couples plasticity in the damage effective stress space can be found in the work of Grassl and Jiràsek (2006).³⁶ While the plastic formulation is improved, along with the calibration of its parameters, the damage driving variable depends on a measure of the accumulation of plastic strain. In this way, the plastic yield surface constitutes a real strength envelope of the material, so that no damage accumulates prior to the peak and therefore, strength is dissociated from elastic characteristics. Although no damage accumulates prior the peak of stress (as evidenced in Fig. 10, where loading-unloading cycles, prior the peak of stress, show no elastic degradation), it is known how inelastic processes begin in this phase as micro cracks start to accumulate. An example of this phenomenon is given by Amann et al. (2011),³⁷ where cumulative acoustic emissions count shows that inelasticity starts before the peak of stress is reached. In the current formulation of the model, such prepeak inelastic processes are implicitly accounted for by the accumulation of plastic strains.

The model is further extended to include true triaxial behavior. Although the equation of the yield surface in the octahedral plane is here presented, it will be analyzed in details in a separate paper. A nonassociated plastic potential is developed in order to avoid overestimation of the dilatant strain in the inelastic phase. The model is implemented into the open source FEM code *Code_Aster*, developed by Électricité de France (EDF) (www.code-aster.org). Validation examples are focused mainly on Opalinus Clay from Switzerland (Mont Terri site for undrained tests and Schlattingen site for undrained tests with pore pressure measurements), although, given the accuracy of the volumetric strain measurements, LaBiche shale from Canada was selected as well. Results demonstrate the ability of the proposed model to account for the prominent characteristics of the deformation process in shales in pure mechanical as well as hydromechanical coupled conditions.

2. Poroelastic coupled hydro-mechanical formulation

We present here the poroelastic theory implemented in *Code_Aster* as described in the work of Plassart et al. (2013),³⁸ which, in this study, constitutes the problem formulation solved in numerical analyses. As *Code_Aster* adopts the sign convention used in solid mechanics, i.e., compressions are negative and tensions positive, we apply this convention in this section only. The remainder of the work uses the convention common in geomechanics, i.e., compressions are positive and tensions negative. In the current work, only undrained analyses at material point level are performed so that the pore pressure field remains uniform and no flow conditions occur. Therefore, only a simplified formulation is proposed, which remains valid for the above-mentioned conditions. The elastic strain increment is driven by the water effective stress increment in saturated conditions with the effective stress equation that writes

$$\sigma_{ij} = \sigma'_{ij} - b p_w \delta_{ij}, \tag{1}$$

where σ_{ij} is the total stress tensor, σ'_{ij} is the effective stress tensor, p_w is the pore water pressure and *b* is Biot's coefficient defined as

$$b = 1 - \frac{K_o}{K_s},\tag{2}$$

with K_o being the undrained modulus of the porous material and K_s the bulk elasticity modulus of the solid skeleton. The variation of porosity $\dot{\phi}$ is a function of the volumetric strain increment $\dot{\epsilon}_{kk}$ defined as

$$\dot{\phi} = (b - \phi) \left(\dot{\epsilon}_{kk} + \frac{P_w}{K_s} \right), \tag{3}$$

where ϕ is the porosity of the medium, i.e., the ratio between pore

volume and total one. The fluid mass m_{ν} is related to fluid mass density ρ_{ν} , initial fluid mass density ρ_{ν}^{0} and initial porosity ϕ^{0} as

$$m_w = \rho_w (1 + \varepsilon_{kk})\phi - \rho_w^0 \phi^0.$$
(4)

Neglecting the volumetric terms, the momentum balance equation of the mixture is defined for a kinematic admissible field $(\bar{\varepsilon}_{ij}, \bar{u}_i, \bar{p}_i)$, in the spirit of the principle of virtual work, as

$$\int_{\Omega} \sigma_{ij} \overline{e}_{ij} dv = \int_{d\Omega} p_i \overline{u}_i ds, \tag{5}$$

while the fluid mass balance as

$$-\int_{\Omega} \frac{dm_{w}}{dt} \overline{p}_{w} dv = \int_{d\Omega} M^{w,ext} \overline{p}_{iw} ds,$$
(6)

where $M^{w,ext}$ is the incoming fluid mass per unit area at the boundaries while p_i is a given traction at boundaries.

3. Plastic damage model

3.1. Isotropic plastic yield surface and hardening internal variables

In the following section the constitutive framework is presented and discussed, along with the yield surface and the hardening equation. The constitutive equation relates stresses with elastic strains as

$$\sigma'_{ij} = (1-d)D^e_{ijkl}\varepsilon^e_{kl},\tag{7}$$

where σ'_{ij} is the nominal water effective stress, *d* is the damage internal variable, D^e_{ijkl} is the rate independent linear elastic stiffness tensor and ϵ^e_{ij} is the elastic strain. The split in the total strain rate tensor $\dot{\epsilon}_{ij}$ between elastic $\dot{\epsilon}^e_{ij}$ and plastic $\dot{\epsilon}^e_{ij}$ strain rate is valid and writes

$$\dot{\varepsilon}_{ij} = \dot{\varepsilon}^e_{ij} + \dot{\varepsilon}^\rho_{ij},\tag{8}$$

The damage effective stress $\tilde{\sigma}'_{ii}$ is defined as

$$\sigma'_{ij} = (1-d)\widetilde{\sigma}'_{ij},\tag{9}$$

We refer to effective stress $\tilde{\sigma}'_{ij}$ as damage effective stress. It is the stress acting in the undamaged part of the solid, where the damage represents the creation of micro-voids inside the material. For further clarification on the physical meaning of damage effective stress and for its derivation, the reader is referred to the work of Lemaître and Desmorat (2005).³⁹ The constitutive relation can be written as

$$\sigma'_{ij} = (1-d)\widetilde{\sigma}'_{ij} = (1-d)D^e_{ijkl}(\varepsilon_{kl} - \varepsilon^p_{kl}), \tag{10}$$

and in rate form becomes

$$\dot{\sigma}'_{ij} = (1-d)D^e_{ijkl}(\dot{\varepsilon}_{kl} - \dot{\varepsilon}^p_{kl}) - \dot{d}D^e_{ijkl}(\varepsilon_{kl} - \varepsilon^p_{kl}).$$
(11)

It can be demonstrated that Eq. (10) can be derived from thermodynamic potentials. According to classical framework for inelastic solids described in Lubliner (1972),⁴⁰ the internal energy*E* at a given point of the solid can be represented as a function of the strain tensor ϵ_{ij} , the entropy per unit volume*S* and a set of internal variables α_i representative of the sequence of events in the material, and can be written as

$$E = E(\varepsilon_{ij}, S, \alpha_i). \tag{12}$$

In case of damage-plastic models, under isothermal conditions, the following expression for internal energy function can be used

$$E(\varepsilon_{ij}, \varepsilon_{ij}^{p}, d) = \frac{1}{2}(1 - d)D_{ijkl}^{e}(\varepsilon_{ij} - \varepsilon_{ij}^{p})(\varepsilon_{kl} - \varepsilon_{kl}^{p}),$$
(13)

and by definition of the state equation $\sigma'_{ij} = \partial_{e_{ij}}E$, one can retrieve the constitutive equation expressed in Eq. (10)

$$\sigma'_{ij} = \partial_{\varepsilon_{ij}} E = (1 - d) D^e_{ijkl} (\varepsilon_{kl} - \varepsilon^p_{kl}).$$
⁽¹⁴⁾

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