Physics and Chemistry of the Earth 33 (2008) S407–S415

Contents lists available at ScienceDirect

Physics and Chemistry of the Earth

journal homepage: www.elsevier.com/locate/pce

On damage modelling in unsaturated clay rocks

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ARTICLE INFO

Article history:
Available online 8 October 2008

Keywords:
Damage
Independent state variables
Poromechanics
Micromechanics
Phenomenological damage model
Multimodal flow model

ABSTRACT

The aim of this paper is to present the main problems encountered in the modelling of damage in an unsaturated quasi-brittle rock mass. Micromechanical damage models are based on a physical definition of damage, related to fracturing. Phenomenological formulations are less straightforward, but offer huge modelling possibilities by means of economical computation processes. Due to the dissipative aspect of damage, the Inequality of Clausius–Duhem (ICD) has to be satisfied. Strain softening and crack localization are regularized by means of a non-local formulation, founded on microstructure concepts, homogenisation and space averaging or gradient-enhancement. In an unsaturated damaged porous medium, suction effects combine with mechanical loading and fracturing, which induces complex couplings. On the one hand, Continuum Damage Mechanics well represents stiffness degradation for dry materials. On the other hand, fracture network models give a good estimation of complex flows. It is difficult to reconcile both theories. A new mixed model, HHMD, is proposed. It is a fully coupled formulation, involving independent state variables.

1. Introduction

This work is part of research dedicated to the study of the Excavation Damaged Zone surrounding galleries for nuclear waste repositories. It is assumed that the material to be modelled is an unsaturated quasi-brittle clay rock.

All of the following statements apply for isothermal conditions. Attention is thus focused on the behaviour of the rock mass before disposal.

Damage modelling involves several theoretical frameworks. The dissipative side of damage involves thermodynamic requirements. Strain softening and crack localization make the problem ill-posed if the damage model is not regularized. Moreover, modelling of the EDZ surrounding deep repositories must take into account saturation variations around the excavation. This involves complex hydro-mechanical couplings, both in the behaviour laws and in the fluid transfer equations.

This work focuses on the main issues to be solved in order to model the hydro-mechanical behaviour of a damaged unsaturated rock mass. A representative sample of existing theoretical frames is reviewed and examined. Then, a new mixed damage model, formulated in independent state variables, is outlined. The first section presents the main keys provided by Continuum Damage Mechanics emphasizing the extension of damage models to unsaturated materials. The second part presents the principles of hydraulic transfer estimation in fracture networks, with emphasis on the introduction of damage in hydraulic transfer models.

2. Continuum-based mechanical damage concepts

Damage of geomaterials is physically related to the fracturing process. However, damage is not always quantified by crack parameters. In some models, more attention is paid to the representation of damage than to its definition. In these particular cases, what is modelled is stiffness degradation and permeability increase rather than crack opening. Damage is thus often an abstract concept, defined indirectly from its influence on the material behaviour. A parallel can be drawn between damage and plasticity models. Damage also involves dissipative processes. Therefore, mechanical damage theories have to satisfy rules of irreversible thermodynamics. Moreover, localization limiters have to be found out in order to avoid the concentration of irreversible strains. However, models dedicated to unsaturated porous media are less common in damage mechanics than in elastoplastic theory. Most of the existing formulations are based on Biot's effective stress concept, which relies on Bishop's stress definition. This latter choice seems not to be valid for unsaturated behaviour, as shown by Fredlund and Morgenstern (1977). One consequence is that it neglects couplings between damage and hydraulics. Another theoretical frame will be proposed.

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doi:10.1016/j.pce.2008.10.006

2.1. Types of models

2.1.1. Micromechanical models

2.1.1.1. Definition and representation of micromechanical damage. The micromechanical approach models the influence of local damage on macro-mechanical behaviour. Damage variables have a physical meaning related to the degradation of elastic properties or to the characteristics of the fracture network. It is assumed that stresses are redistributed due to a decrease of the effective material area. Stress–strain relationships are thus written in terms of effective variables. The effective stress is the stress that develops in the fictive undamaged counterpart of the system (de Borst et al., 1999). Its definitions require the use of a fourth-order effective-stress operator (Hansen and Schreyer, 1994):

$$\underline{\underline{\hat{\sigma}}} = \underline{\underline{\underline{\underline{M}}}}(\Omega) : \underline{\underline{\sigma}} \tag{1}$$

where the damage variable Ω can be a tensor. The effective stress concept is often combined with the Principle of Equivalent Elastic Energy (PEEE) to compute the damaged rigidity tensor $\underline{\underline{\underline{\underline{D_e}}}}(\Omega)$. As recalled in (Hansen and Schreyer, 1994), this approach postulates that the elastic energy of the intact material subjected to the effective stress $\underline{\underline{\hat{\sigma}}}$ is equal to the elastic energy of the damaged material subjected to the real stress $\underline{\underline{\sigma}}(W_e(\underline{\underline{\hat{\sigma}}}, \Omega = 0) = W_e(\underline{\underline{\sigma}}, \Omega))$, which leads to the equality:

$$\underline{\underline{\underline{\underline{D_e}}}}(\Omega) = \underline{\underline{\underline{\underline{M}}}}(\Omega)^{-1} : \underline{\underline{\underline{\underline{D_e^0}}}} : \underline{\underline{\underline{\underline{M}}}}(\Omega)^{-T} \tag{2}$$

The definition of an effective stress provides a framework to determine the damaged mechanical properties of the material. However, damage remains an abstract notion, represented by its influence on behaviour laws. That is why in some models, damage is also given a physical meaning, generally related to fracturing. A common approach consists in gathering cracks into "families" of close orientations (Swoboda and Yang, 1999b; Shao and Rudnicki, 2000; Shao et al., 2005a). Following the principle of spectral decomposition of Ortiz (Ortiz, 1985), a second-order damage variable is defined as follows:

$$\underline{\underline{\Omega}} = \sum_{i=1}^{3} d_i \underline{n_i} \otimes \underline{n_i} \tag{3}$$

Equality (3) infers that the material is fractured in three principal directions n_i whose importance is weighed by the crack densities d_i. Definition (3) assumes that cracks are non-interacting. Bazant (1991) proposed to take fracture interactions into account by defining crack opening as a function of the energy release rates of every crack of the Representative Elementary Volume (REV), weighed by interaction coefficients specific to each pair of fractures.

2.1.1.2. Non-locality of micromechanical damage theories. Since the micromechanical methods update macro-data using micro-data, the theory is non-local. Bazant gave micromechanical evidences of the need for a non-local formulation in Bazant (1991). Generally speaking, a non-local model is based on a theoretical frame requiring the introduction of an internal length parameter. This length can be related to material properties, such as grain size. Bazant and Jirasek (Jirasek, 1998; Bazant and Jirasek, 2002) distinguish microstructure, differential and integral theories. In microstructure models, which will be studied in the following subsection, each material point is seen as a deformable particle endowed with degrees of freedom defined at the microscale. The structure of the material is thus enriched. Differential frameworks are based on the introduction of the gradients of local or non-local variables in the constitutive equations. Some of them are based on the theory of microstructure. For example, in second grade models, the internal power density is assumed to depend not only on deformations, but also on the gradient of deformations. It is the representation of a particular micromorphic medium of degree one expressed in a first gradient frame, in which macrodeformations and microdeformations are set equal (Germain, 1973b; Vardoulakis and Sulem, 1995; Chambon et al., 2004). In some other differential non-local theories, the spatial gradients are not related to microstructure. Zbib and Aifantis (Al-Holo Al-Radi, 2005) introduced the Laplacian of plastic deformations in a softening behaviour law. In their model, the deviatoric stress depends on the local deviatoric stress and on the first terms of a Taylor's series. In other models, an averaged state variable is replaced by the first terms of the Taylor series of the corresponding local quantity, leading to the introduction of a second-gradient in the constitutive laws (Lasry and Belytschko, 1988; de Borst et al., 1999; Kuhl and Ramm, 1999; Askes et al., 2000; Askes and Sluys, 2002; Pamin, 2005; Isaksson and Hägglund, 2007). The weighing coefficients of the gradient terms depend on a material length related to the dimension of the zone of influence of local damage. Integral formulations (Bazant and Ozbolt, 1990; Bazant, 1991; de Vree et al., 1995; Jirasek, 1998) also involve the spatial averaging of material properties on the neighbourhood of the observed point. As explained in the review paper by Bazant and Jirasek (Bazant and Jirasek, 2002), a local state variable $f(x)$ is replaced by a spatial average $\bar{f}(x)$:

$$\bar{f}(x) = \int_{V_{tot}} \alpha(x, \xi) f(\xi) \mathrm{d}\xi \tag{4}$$

where V_{tot} denotes the volume of the entire system (and not just the REV). The attenuation function $\alpha(x, \xi)$ represents the decreasing distance of influence of a given state variable in space. The use of decreasing weighing functions allows the averaging integral (4) on the whole volume of the system V_{tot}.to be calculated. It is thus not necessary to define representative volume elements explicitly, because homogenisation is already included in the computation process. In order to guarantee the absence of residual stresses after damage, Jirasek (1998) recommends the introduction of either the non-local deformation, the non-local energy release rate, or the non-local damage deformation into the constitutive relations.

2.1.2. Energetic approaches

Energetic considerations are particularly suited to model dissipative phenomena such as damage and plasticity. Thermodynamic potentials are given specific forms. In many models, the expression for the free energy is chosen depending on the expected behaviour law (Svedberg and Runesson, 1997; Homand-Etienne et al., 1998; Shao and Rudnicki, 2000; Menzel and Steinmann, 2001; Shao et al., 2005a,b). Formulations starting from the Principle of Virtual Power (Frémond and Nedjar, 1996; Pires-Domingues et al., 1998; Nedjar, 2001; Zhao et al., 2005) can encompass an enrichment of the material's structure, implying the definition of higher-order stresses and specific boundary conditions.

2.2. Thermodynamic framework

An overview of continuum thermodynamics is given in Hansen and Schreyer (1994) and Collins and Houlsby (1997). At a local point x, the internal energy U of the studied system depends on the entropy $S(x)$, strain variables $\underline{\underline{E}}(\underline{x})$ and on parameters representing irreversible or dissipative processes $\upsilon_i(x)$. The first law of thermodynamics means that the variation of the internal energy is equal to the work of deformation minus the heat provided to the exterior of the system:

$$\dot{U}(S(\underline{x}), \underline{\underline{E}}(\underline{x}), \upsilon_i(\underline{x})) = \underline{\underline{\sum}}(\underline{x}) : \underline{\underline{\dot{E}}}(\underline{x}) - \underline{\nabla} \cdot \underline{q}(\underline{x}) \tag{5}$$

$\underline{\underline{\sum}}(\underline{x})$is the generalized stress tensor, and $\underline{q}(\underline{x})$ is the heat flux vector. Due to the occurrence of irreversible processes, entropy production