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Probabilistic optimization of a continuum mechanics model to predict differential stress-induced damage in claystone

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ABSTRACT

Phenomenological modeling of anisotropic damage in rock raises many fundamental thermodynamic and mechanical issues. In this paper, the maximum likelihood method is used to analyze the performance of the Differential Stress Induced Damage (DSID) model recently formulated by Xu and Arson [1]. The stress/strain relationship is a nonlinear function of parameters including unknown constants (i.e., damage constitutive parameters) and known variables (e.g., elastic parameters and controlled stress state). Logarithmic transformation, normalization and forward deletion are employed, in order to find the optimum number of constitutive parameters, as a trade off between accuracy and simplicity. For Eastern France claystone subject to deviatoric stress loading (e.g., triaxial and proportional compression loading), it is found that (1) only one damage parameter (a_2) is needed in the expression of the free energy to predict stress/strain curves; (2) a_2 controls the deviation of the current principal directions of stress to the principal directions of damage; (3) model parameters involved in the damage criterion can be related to a_2. As a result, a_2 is the only parameter needed to model differential-stress induced damage in Eastern France claystone. It is also shown that within the set of assumptions made in this study, the DSID model is not sensitive to the initial damage threshold C_0, except for $C_0 > 10^6$ Pa, a range of values in which only one constitutive parameter becomes insufficient to predict the stress/strain curves of damaged claystone. Coupling probabilistic calibration and optimization methods to numerical codes promises to allow adapting the complexity of anisotropic damage models to different rocks and stress paths.

1. Introduction

At present, 85% of the energy power consumed in the world is produced by fossil fuel combustion [2,3], which has raised increasing interest in renewable energy technologies, non-conventional oil and gas reservoirs, and nuclear power. Innovative nuclear fuels and reactors depend on the economical and environmental impacts of waste management [4]. Disposals in mined geological formations are viewed as potential consolidated storage facilities before final disposition [5]. Rock damage is therefore a core issue in energy production (e.g., hydraulic fracturing [6–8] and geothermal energy extraction [9–11]) , energy storage (e.g., Compressed Air Energy Storage [12–14]) and waste management (e.g., nuclear waste disposals [15–19] and carbon capture [20–23]). Continuum Damage Mechanics (CDM) provides an efficient framework to bridge the failure plane scale with the pore and the crack scale. Damage is a thermodynamic variable used to (1) represent crack initiation, propagation and coalescence in rock; and (2) model the subsequent changes of rock mechanical, physical and chemical properties at the scale of a Representative Elementary Volume (REV) [24,25].

CDM-based models have an important practical interest for engineers, and are based on rigorous closed-form formulations. However, the difficulty to determine the magnitude of material parameters is overwhelming. The maximum likelihood method has been widely used in the past to find the optimum values of unknown parameters in probabilistic models. This method can also be employed to determine the standard error associated with a model, in order to assess the accuracy and reliability of this model. Also, it is possible to establish a procedure to remove unnecessary parameters or combine the ones which are correlated with each other. As a result, simpler models can be obtained, with fewer parameters. The maximum likelihood method also provides some insight into the relative importance of parameters in real physical problems. For instance, Ledesma et al. [26] used this method to find a constitutive model for soft biological tissues. Jung et al. used a Bayesian updating method (based on the maximum likelihood method) to find a constitutive law in a simplified unified compression model for soil deposits [27], and to improve soil classifications [28]. Medina-Cetina and Arson [29] and Arson and Medina-Cetina [30] used the Bayesian paradigm to calibrate a damage mechanics model for rock, and to interpret the mathematical independence of the constitutive parameters. Boyce and Chamis [31] used both the maximum entropy principle and the

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maximum likelihood method to establish probabilistic constitutive relationships for cyclic material strength models. Gardoni et al. [32,33] used a total of 384 strand test specimens to study self-consolidated concrete exposed to various void, moisture, and chloride concentration conditions. Using experimental results and the maximum likelihood method, a probabilistic model was developed. Tsuchiya et al. [34] estimated the Weibull modulus of brittle materials using the maximum likelihood method. Instead of using a linear regression method, Huang et al. [35] employed the maximum likelihood method to predict concrete compressive strength using ultrasonic pulse velocity and rebound number. Trejo et al. [36] and Pillai et al. [37] identified and quantified important parameters influencing the corrosion and tension capacity of strands in post-tensioned bridges.

In the work presented in the following, the maximum likelihood method is used to analyze the performance of the Differential Stress Induced Damage (DSID) model recently formulated by the authors [1], with a particular focus on the stress/strain response of Eastern France claystone subjected to deviatoric stress loading. The main mineral and mechanical properties of the claystone under study are summarized in Section 2, along with the main constitutive models proposed so far. Section 3 outlines the thermodynamic framework of the DSID model, and provides the state-of-the-art of the methods available to calibrate the related damage constitutive parameters. The proposed probabilistic model is presented in Section 4: known variables and unknown parameters are identified first, the implementation of the maximum likelihood method is explained then, and a probabilistic strategy is finally established for the use of the DSID model. Section 5 highlights the need for a parameter calibration, and methodically presents the optimization procedure used in this study. Section 6 discusses the significance of the results, and provides further performance assessment of the DSID model.

2. Overview of the characterization and modeling of claystone

2.1. Mineral composition and physical properties

Claystone is a mudrock – a class of fine grained siliciclastic sedimentary rocks. More than 50% of the composition of claystone is clay-sized particles, less than 4 μm in size. Claystones contain quartz, feldspar, iron oxides, and carbonate minerals (in variable proportion, depending on the geological formation). In general, claystones tend to have low permeability but high mechanical strength. Clay minerals such as smectite and illite are very sensitive to the saturation degree, which can result in pronounced plastic deformation [38]. The behavior of claystone is more brittle when calcite content increases, and inversely becomes more ductile when the quantity of clay elements increases [39]. There is also a strong dependence of the mechanical behavior on the confining pressure, marked by a transition from a fragile towards a ductile behavior [40]. Table 1 summarizes the mineral and physical characteristics of claystones.

2.2. Experimental characterization

Claystones are sedimentary rocks: they are structured in layers by the process of deposition. At the microscopic scale, anisotropy is manifested by the sliding of clay sheets and the twilling in a few large calcite grains – two phenomena which are related to the distribution of voids in the clay matrix. At the scale of the laboratory sample (Representative Elementary Volume, REV), claystone anisotropy can be seen during a hydrostatic compression loading (e.g., [39]): the response of the material to the applied loading exhibits a different deformation in the axial and radial directions. In order to capture the resulting intrinsic anisotropy of

Table 1
Summary of the mineral and physical characteristics of claystone.

Origin	Physical properties						
	Minerals	Density	Porosity	Permeability	Water content	Saturation	Grain size
Meuse/Haute Marne (Paris Basin)	Calcite: 27 ± 9%; quartz: 23 ± 4%; clay matrix: 45 ± 7%. Some accessory minerals are subordinate feldspars, pyrite, and iron oxides, about a volumetric fraction of 5%. The clay mineral composition is relatively constant at 65% I/S (illite/smectite interstratified minerals), 30% illite and 5% kaolinite and chlorite	The bulk, dry and grain density are respectively 2.41 ± 0.06, 2.27 ± 0.03 and 2.65 g/cm^3	11.8 ± 1.6%	$10^{-19}-10^{-20}$ m^2	6.2 ± 1.38%	95 ± 1.1%	The average size of calcite and quartz grains is generally less than 200 μm
[39] Eastern France	Quartz: 52%; calcite: about 28%; clays (smectite, illite, kaolinite and chlorite)			Intrinsic permeability 10^{-20} m^2			
	Calcite: 20–40%, quartz 20–30%, clays 40–55%		11.5–12%		4–5.7%		
	Calcite: 25–55%, quartz 20–30%, clays 35–55%		11–13.5%		4–7%		
	Calcite: 25–35%, quartz 15–20%, clays 45–60%		12%		4–7%		
[41] Eastern France				Intrinsic permeability 10^{-21} m^2 Intrinsic permeability $k=10^{-21}$ m^2, $\mu=10^{-3}$ Pa s			