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Sensitivity analysis and parameter identification of a time dependent constitutive model for rock salt

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ABSTRACT

The tendency to shift from fossil and nuclear energy sources to renewable energy carriers has increased during the past couple of decades. Subsequently, development of effective energy storage systems has become more attractive. Nowadays, caverns excavated in rock salt formations are recognized as the appropriate places for underground storage of energy in the form of compressed air or hydrogen. Accurate design of these underground cavities requires suitable numerical simulations employing appropriate constitutive models to describe the material behavior of rock salt under various geological conditions. It is obvious that to have a realistic numerical simulation, it is essential to have a comprehensive knowledge concerning the unknown material parameters and their influence on the calculation results. In this paper, a time dependent model is selected to describe the mechanical response of the rock salt around the cavern. This model is implemented in a finite element code and its application in numerical modeling of salt caverns is illustrated. In addition, global sensitivity analysis is used to investigate the influence of material parameters on the mechanical behavior of the salt cavern. Finally, inverse analysis of the synthetic data is performed to identify the material parameters of the selected model. The applied global sensitivity and inverse analysis algorithms employ metamodeling technique in order to reduce the time which is needed for these computationally expensive calculations.

1. Introduction

The low permeability and adequate thermal and mechanical properties of rock salt have made it a suitable choice for the underground storage of compressed air, CO_2 and H_2. Accurate design of the underground openings in the rock salt formations is possible if a proper constitutive law is used to describe the material behavior of salt. Numerous investigations have been carried out during the past couple of decades in order to find an adequate description for the mechanical behavior of rock salt (e.g. [1–4]). In this paper, the Lubby2 model developed by Heusermann in [5] is implemented in the finite element code Code–Bright to simulate the time dependent behavior of rock salt around the underground cavities. Code–Bright (COupled DEformation BRIne, Gas and Heat Transport) [6] is a program that allows for thermo-hydro-mechanical analysis in geological media. It consists of a finite element program developed at the Department of the Geotechnical Engineering and Geosciences of the Technical University of Catalonia (UPC). In the numerical section, a typical cylindrical salt cavern is modeled based on Lubby2 material model. Then, the effect of three parameters of the employed constitutive model on the calculation results is

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investigated by using two global sensitivity analysis (GSA) methods. Finally, inverse analysis of synthetic data is performed to identify the material parameters of the selected constitutive model. For solving the optimization problem within the back analysis in this paper we used genetic algorithm. Both the sensitivity and the back analyses are realized employing metamodeling technique as a reliable tool to manage computationally expensive models. Although applications of meta-models, surrogate models or emulators to sensitivity and inverse modeling are widely reported, we emphasized here on such an application to a time dependent constitutive model as part of an engineering problem whose numerical simulation may be costly with respect to computational time. Employment of model emulation is well established technique for sensitivity analysis with application to environmental modeling. Here we give only some example references and a thorough recent review on metamodeling may be found in [7] and on global sensitivity methods in e.g. [8–10]. In Ref. [11], the Gaussian process metamodel has been applied to perform variance based sensitivity analysis and to derive analytical expressions for the Sobol indices, an approach to sensitivity index estimation using meta-models and bootstrap confidence intervals is described in [12]. Combining screening and metamodel based methods was also shown to be an efficient approach to sensitivity analysis in [13]. A methodology for GSA combining distribution-based sensitivity measures and emulators is proposed in [14]. Gaussian process and POD decomposition were used in [15] to build a surrogate model with application to sensitivity analysis for spatio-temporal numerical simulators, particularly for an atmospheric dispersion process simulator. Meta-model-based importance sampling is discussed in [16] with application to structural safety and failure probability analysis. State dependent parameter modeling is applied in [17] to estimate the variance based sensitivity indices and the procedure is shown to be conceptually simple and very efficient. We are not going to present here an extensive survey on the literature devoted to development of algorithms and applications of metamodeling and sensitivity analysis but only gave some examples that encouraged us to apply this technique in our research.

2. Mechanical behavior of rock salt

Polycrystalline halite rocks (rock salt) consists of grains of halite (NaCl), with diameter between 0.01 mm and several dm, containing impurities in solid solution, secondary mineral phases and fluids trapped in grain boundaries or in pores [18]. When a constant load is applied to the rock salt, a time dependent ductile deformation without any visible macroscopic fracture is observed. This time dependent behavior is highly affected by the magnitude of the applied load as well as the environmental factors like temperature and humidity. In case the applied load or temperature is too high, the micro-cracking, inter-granular slip as well as crystal plasticity occur. Numerous experiments on rock salt samples performed by several researchers show that there exist a zone in stress space whose boundary separates the ductile behavior from the brittle response (see [1]). Caverns excavated in rock salt should be designed in a way that the stress state for all the points around the cavern remains inside the ductile zone. In this paper, the Lubby2 model is used to describe the time dependent ductile response of the rock salt around the cavern under quasi-static geological loading [5]. This model considers the strain rate as a sum of two parts, i.e. elastic strain rate $\dot{\varepsilon}_{ij}^{e}$ and the visco-elastic strain rate $\dot{\varepsilon}_{ij}^{ve}$.

$$\dot{\varepsilon}_{ij} = \dot{\varepsilon}_{ij}^{e} + \dot{\varepsilon}_{ij}^{ve}. \tag{1}$$

Fig. 1 shows the sketch of the employed rheological model. The elastic strain is obtained using the generalized Hooke's law. The material characteristic of the dashpots and springs in this model are stress dependent. The visco-elastic strain rate in this model is divided into two parts: (1) transient phase (ε^{tr}) (2) steady-state phase (ε^{ss}). The following equations define the visco-elastic strain rate:

$$\begin{cases} \dot{\varepsilon}_{ij}^{ve} = \dot{\varepsilon}_{ij}^{tr} + \dot{\varepsilon}_{ij}^{ss}, \\ \dot{\varepsilon}_{ij}^{tr} = \dfrac{3}{2}\dfrac{1}{\bar{\eta}_k}\left(1 - \dfrac{\bar{G}_k \varepsilon^{tr}}{q}\right) S_{ij}, \\ \dot{\varepsilon}_{ij}^{ss} = \dfrac{3}{2}\dfrac{1}{\bar{\eta}_m} S_{ij}. \end{cases} \tag{2}$$

where S_{ij} is the (ij)th element of the deviatoric stress tensor and ε^{tr} represents the equivalent transient strain. $\bar{\eta}_k$ and $\bar{\eta}_m$ correspond to Kelvin and Maxwell viscosity coefficients respectively and $\bar{G}_k$ represents the Kelvin module. The stress dependency of these coefficients can be described by using the following equations.

$$\bar{\eta}_k = \eta_k \exp\left(k_2 q\right), \qquad \bar{\eta}_m = \eta_m \exp\left(mq\right), \qquad \bar{G}_k = G_k \exp\left(k_1 q\right). \tag{3}$$

$\eta_k, \eta_m, G_k, k_1, k_2$ and m are constant material parameters and q represents the equivalent deviatoric stress ($q = \sqrt{2/3 S_{ij} S_{ij}}$).

2.1. Integration of constitutive equations

In this paper, implicit integration scheme has been utilized to obtain the stress increment. Using the generalized Hooke's law, the stress increment at time $t + \Delta t$ is calculated as follows:

$$d\boldsymbol{\sigma}_{t+\Delta t} = \mathbf{C}(d\dot{\boldsymbol{\varepsilon}}_{t+\Delta t} - d\dot{\boldsymbol{\varepsilon}}_{t+\Delta t}^{ve})\Delta t, \tag{4}$$