THM Modelling of Expansive Clays incorporating Uncertainty Quantification

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Introduction

The design of repositories for high level nuclear waste involves simultaneous changes in the thermal, hydrologic and mechanical fields generally requires the use of coupled Thermo-Hydro-Mechanical (THM) formulations. The THM formulations are generally composed of a number of balance equations for porous media; a set of constitutive equations; and equilibrium restrictions as components of this process. To simulate these behaviors, numerical models are implemented with a number of parameters describing the intrinsic thermal, hydraulic and mechanical behaviors. The parameters are often determined by using deterministic approaches by fitting a model over experimental observation (Olivella, et al. 1994, 1996). However, certain uncertainties exist over determining the parameter value, due to which the model output would not fully capture actual observations. This work explores a methodology of capturing these uncertainties using probabilistic calibration methods, particularly using Bayesian paradigms and Markov chains. The results of using such methods are then contrasted with the original numerical results and the actual observations.

Experiment and Formulation

To study the behavior of near field for a High Level Waste (HLW) repository in crystalline rock, FEBEX (Full-scale Engineered Barriers Experiment) project was undertaken. It was based on the Spanish reference con-cept for disposal of placing the waste canisters horizontally in drifts, driven in crystalline rock, and surrounded by a clay barrier constructed from highly-compacted bentonite blocks (ENRESA, 2006). The experimental work consisted of three main parts: (1) an in situ test, under natural conditions and at full scale, performed at the Grimsel Test Site (GTS, Switzerland); (2) a mock-up test, at almost full scale, performed at CIEMAT facili-ties (Madrid); and (3) a series of laboratory tests to complement the information from the two large-scale tests. As a part of laboratory test, samples were collected from the bentonite blocks and tested for their intrinsic prop-erties. The physico-chemical properties of the bentonite, as well as its most relevant thermo-hydro-mechanical and geochemical characteristics were summarized in the final reports of the project (ENRESA, 2006).

In order to simulate the behavior of the barrier a fully coupled THM formulation was developed (Sanchez et al., 2012). For simplicity, no chemical actions have been considered here. The details of the balance equations, constitutive equations and the equilibrium restrictions have been discussed in detail elsewhere (Sanchez et al., 2012).

Parametric analysis

The mathematical framework used in the initial modeling has huge variation with the experimental observa-tions. Assigning a deterministic value to the parameter to produce the output response may not be in agreement with the actual response. Hence, the material random responses and local effects are to be considered in the as-sessment of the model parameters and their variations need to be calibrated. The probabilistic calibration method proposed by Medina-Cetina (2007), which uses Functional Bayesian (FB) is then followed to quantify the THM response of bentonite clay used as material in nuclear waste repository. The randomness of the pa-rameters along with their uncertainty is captured and full description of the parameters is obtained using the Bayesian formulation. The method uses a-priori knowledge of the constitutive parameters (prior) updated with the predictive model performance (likelihood); yielding a joint Probability Density Function (PDF) known as the posterior which can be interpreted as the probability of occurrence of the parameter given the experimental ob-servations. Integrating the posterior is a complex process especially involving multivariate distribution function. To avoid this situation, Monte Carlo integration is adopted for integration of posterior using the rules of Markov Chains (MCMC) and Metropolis-Hastings (M-H) (Metropolis et al., 1953).

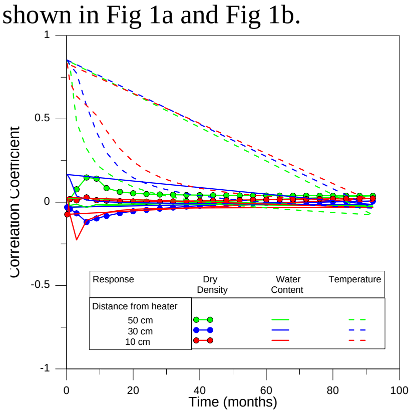
The parameter distributions were generated specifically for thermal conductivity laws and retention curves used to ascertain the uncertainty in the THM model response by repeatedly evaluating the model using each set of parameters, so that the output response is estimated in the form of probability distribution functions (PDF). In the present work, the uncertainty in THM modeling of the engineered barrier, due to variability in thermal and hydraulic parameter, is assessed. The analysis is performed using the finite element program CODE_BRIGHT (Olivella et al., 1996) which is based on the THM formulation.

Assessment of THM model response

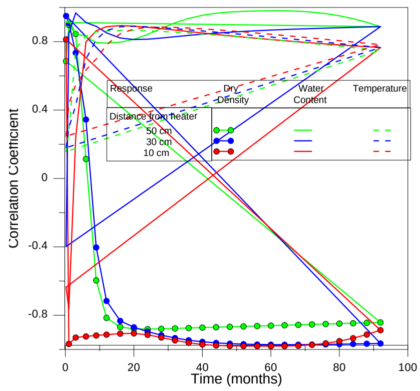
The experiment simulation of the barrier consisted of a cylindrical cell of length 60 cm, diameter 7 cm (Villar et al., 2008). Inside the cells, a series of six blocks of FEBEX bentonite compacted to dry density 1.65 g/cm3 were piled up vertically similar to compacted bentonite blocks used in the HLW repository in crystalline rock (ENRESA, 2006). The bottom surface of the material was heated at 100°C and the top surface was injected with granitic water. A series of seven such tests were performed for different periods of time (two of 0.5-year du-ration, two of 1 year duration, two of 2 years duration and one of 7.6 years duration). This setup was modelled using 1D finite element mesh with 50 linear elements to represent the one dimensional cell. These elements were assigned the properties of compacted bentonite used in the experiment and the same boundary conditions are maintained.

Each set of parameters was propagated into the model and the output of response was observed. The statis-tics of the vector of each parameter passed into the model was maintained same as that of their respective par-ent distribution set. The response output from the model was then assembled and analyzed for spatial-temporal statistics. The uncertainty is classically expressed in terms of first order inferences which include mean, and standard deviation. Cumulative distribution functions (CDF) were used by providing probability estimates for different levels of performance.

The temperature response was in agreement with the model response, although it failed to capture the tem-poral evolution accurately. The model predicted the trend of water content, but shows variation with the actual values. The uncertainty in thermal conductivity has no influence; to add, the model response is under predicted. The uncertainty in predicting the dry density at the initial stages persisted even after propagating the variation in both thermal and hydraulic parameters. This suggests that there could be some other parameters whose varia-tion has to be taken into consideration. Correlation coefficient between the output response at different loca-tions and time are shown in Fig 1a and Fig 1b.



a) Response thermal conductivity of dry soil



b) Response and the intrinsic permeability

Fig 1. Correlation coefficient between the output response at different locations with time

References

ENRESA Full-scale Engineered Barriers Experiment. Final Report 1994-2004. Publicación Técnica (2006). Madrid. 590 pp

Sánchez, M., Gens, A. and Olivella, S. ‘THM analysis of a large-scale heating test incorporating material fabric changes’, International journal for numerical and analytical methods in geomechanics. John Wiley & Sons, Ltd, 36(4), (2012), pp. 391–421. doi: 10.1002/nag.1011

Medina-Cetina, Zenon. "Probabilistic calibration of a soil model." PhD diss., (2007). Johns Hopkins University

Olivella, Sebastià, A. Gens, J. Carrera, and E. E. Alonso. "Numerical formulation for a simulator (CODE_BRIGHT) for the coupled analysis of saline media." Engineering computations 13, no. 7 (1996): 87-112

Olivella, S., J. Carrera, A. Gens, and E. E. Alonso. "Nonisothermal multiphase flow of brine and gas through saline media." Transport in porous media 15, no. 3 (1994): 271-293

Metropolis, Nicholas, Arianna W. Rosenbluth, Marshall N. Rosenbluth, Augusta H. Teller, and Edward Teller. "Equation of state calculations by fast computing machines." The journal of chemical physics 21, no. 6 (1953): 1087-1092

Villar, M. Victoria, and Antonio Lloret. "Influence of dry density and water content on the swelling of a compacted bentonite." Applied Clay Science 39.1-2 (2008): 38-49