# **Using Statistical Methods for Rock Parameter** Identification to analyse the THM Behaviour of Callovo-**Oxfordian Claystone**

# Introduction

To study the thermo-hydro-mechanical effects of the thermal transient phase on the clay host rock of a deep repository, ANDRA (the French National Radioactive Waste Management Agency) performed an in-situ heating test called TED experiment. This experiment was the second one carried out in the Meuse/Haute-Marne Underground Research Laboratory focusing on determining the thermo-hydromechanical behavior of the Callovo-Oxfordian claystone. The aim of the TED experiment was to measure the temperature, deformation, and pore-pressure field evolution around heaters and to backanalyze the thermo-hydro-mechanical properties of the Callovo-Oxfordian claystone. The TED experiment was also designed to study the evolution of the damaged zone due to heating. The analyses of the TED experiment results will help to calibrate the numerical models that will be applied to the French disposal cell concept (ANDRA 2005). An automatic parameter identification process has been applied, and the results are presented in this paper.

## The heating experiment

The test set-up consists of 3 heater boreholes and 21 instrumented observation boreholes. Each heater is 4 m long and generates a thermal power of 1500 W. The distance between the heaters is 2.6 m in order to approximate the geometry of the planned disposal cells. The surrounding boreholes were strategically located to take into account the anisotropic THM behavior of the claystone (Figure 1). There are 12 boreholes for pore pressure measurements, 9 boreholes for temperature measurements, and 2 boreholes for deformation measurements. To optimize and simplify the inverse problem analysis, special attention was paid to the reduction of uncertainties regarding the sensors' locations in the boreholes.



*Figure 1: Location of boreholes in the TED experiment.* 

The central heater was activated on January 25, 2010, starting with a relatively low heating power of 150 W. Subsequently, the heating power was increased to 300 W and finally to 600 W. Each step was about four months long. After one year, the two surrounding heaters were activated, and the same heat load was applied.

# Methodology for rock parameter identification

Dynardo developed a 3D THM simulator by coupling ANSYS parametric modeling and implicit FEM simulation environment with multiPlas (DYNARDO 2010). To calibrate the numerical model to the in-situ experimental results, the software tool optiSLang (DYNARDO 2015) was coupled to the THM simulator for CAE-based sensitivity analysis and optimization. The uncertain input parameters for the numerical model from the best in-situ and laboratory data available need to be calibrated to the in-situ measurements. Here, efficient ways of performing sensitivity analyses to identify the most important input parameters and to calibrate the numerical models to experimental data become important. With optiSLang, we perform numerical sensitivity studies for nonlinear problems using optimized stochastic sampling strategies. In Figure 2 the workflow for parameter calibration is shown.



Figure 2: Work flow of parameter calibration.

With Latin Hypercube sampling, the design space will be scanned followed by statistical measurements of the importance of individual model parameters using the Coefficient of Prognosis (CoP). The CoP measures the amount of response parameter variation which results from the input variation of every single uncertain parameter. The basis of this determination measurement is the correlation analysis including linear and nonlinear correlation hypotheses. The detection of nonlinear correlations that have a large number of uncertain parameters with a minimum number of design evaluations is conducted by the Meta-model of Optimal Prognosis (MOP) algorithm (DYNARDO 2015).

## Numerical model

In view of calculation time, the geometric model size and mesh discretization of the model have to be chosen carefully because dozens of simulations are needed for calibration procedure. At the same time, the boundary conditions have to be placed far enough so they have only insignificant influence



Figure 3: a) Model domain.

b) FE Model

on the results. Therefore, different model sizes and discretization levels were tested to find a model that shows the best compromise between accuracy of the results and adequate calculation time. The total model domain and the mesh are shown in Figure 3a and 3b. In total, 300.000 elements are used. The model domain contains the tunnel and the niche at the URL with shotcrete surfaces, the three boreholes with the heaters, and two observation boreholes intended for mechanical deformation measurements. The latter act as hydraulic sinks in the domain and have therefore been considered in the model.

#### Simulation of the heater test - Temperature evolution

The basic THM simulation carefully modeled the experiment including the tunnel excavation, the heater boreholes, and all heating phases. The thermal analysis does not depend much on hydraulic or mechanical processes but is the driving force for all the hydro-mechanical processes in the experimental area. Therefore, the thermal rock material properties were calibrated separately at the beginning to ensure a good representation of the temperature evolution in the model. The initial input parameters as starting values for the parameter identification were taken from laboratory investigations on drill core samples and are given in (Jobmann 2010). In Figure 4 (left), the comparison of measured and calculated temperature evolutions for three selected sensors after parameter identification is shown. The good fitting is evident.

## Simulation of the heater test - Porewater pressure evolution

For the sensitivity analysis, 80 designs were generated. The important results of the sensitivity analysis are CoP values (Coefficient of Prognosis) which show the significance of input parameters. The CoPs at the beginning of heating (time 0) indicate that during tunnel excavation and borehole drilling for the measurement points 1251, 1252, 1253 and 1255, which are located in the so-called "reference plane" at a depth of 14 m, the most important parameter is permeability parallel to bedding plane. For measurement points 1258 and 1259, which are located out of the reference plane, the most important parameter is permeability perpendicular to bedding plane. At some points, especially 1251, which is very close to the middle heater, the important influence of the strength parameters  $\varphi_{g}$ .  $c_{g}$  (effect of plasticity) can be seen. The CoPs at time 295 and 400 days identify the important input parameters regarding the maximum pore pressure during the 3<sup>rd</sup> heating phase and the end value of the 3<sup>rd</sup> heating phase. Here, the factor of the thermal expansion function (pore water expansion)  $\alpha_{f,factor}$ , the porosity *n*, and the Biot modulus *M* are very important as well.

For solving the calibration problem of minimizing the difference between simulation and measurement, two optimization algorithms were used. Starting from the best design of the sensitivity analysis, we used optiSLang's adaptive response surface method. This methodology follows the main trends to improve the fitting. In a second step, we used evolutionary algorithms for further local refinement of parameter values. Figure 4 (right) compares the results of the best design after calibration with the measurements at a selected borehole. The pore pressures fit quite well at this location and represent a good fitting quality for horizontal and vertical flow.



Figure 4: Comparison of calculated best design with measured signal: left) temperature evolutions for three selected sensors. right) relative pore pressures versus time at TED 1258

As result of the parameter identification, the following parameters of the Callovo-Oxfordian claystone were identified:

density: 2333 kg m<sup>-3</sup>, specific heat capacity: 695 J kg<sup>-1</sup> K<sup>-1</sup>, horizontal thermal conductivity: 2.02 W m<sup>-1</sup> K<sup>-1</sup>, vertical thermal conductivity 1.37 W m<sup>-1</sup> K<sup>-1</sup>, friction angle (intact): 28.79°, cohesion: 3.79 MPa, friction angle (bedding plane): 23.54°, ratios of residual to initial strength factors (intact): friction angle 0.84, cohesion 0.444, porosity: 0.16, biot modulus: 3.9 GPa, biot coefficient: 0.65,

constants of permeability functions for an exponential relation between intrinsic permeability and stress state (parallel to bedding plane  $k\sigma, x = k\sigma, y$  and perpendicular to bedding plane  $k\sigma, z$ ):

$$k_{\sigma,z} = k_{\sigma,n} = k_{0,n} \times \left(\frac{\sigma_{m,h}}{\sigma_0}\right)^{-n_n} \qquad \qquad k_{\sigma,x} = k_{\sigma,y} = k_{0,p} \times \left(\frac{\sigma_z}{\sigma_0}\right)^{-n_p}$$

where  $\sigma 0 = 1$  MPa, k0,p = 5.87E-19 m<sup>2</sup>, n<sub>p</sub> = 1.07871, k0,n = 1.5E-20, n<sub>n</sub> = 0.15363

## **Evaluation and conclusions**

Using ANSYS and multiPlas, a 3-dimensional parametric THM simulator was set up that could be calibrated to in-situ measurement results of a heater experiment. A high numerical efficiency of the simulator was achieved. The simulator needed 32 hours to calculate one design of the calibration process running in-situ stress generation and three heating periods with an up-to-date dual core workstation in 2011.

OptiSLang's functionality for sensitivity analysis and calibration dealing with a large amount of uncertainties was linked to the simulator and, with a correlation analysis the main rock parameters were identified, making visible the mechanism of how the rock parameter variation effects important THM simulation results. This knowledge is essential for defining appropriate boundary conditions for the calibration, appropriate parameter space, constraints, and an objective function. Depending on the number of important parameters that can be calibrated and on the non-linearity of the calibration results, we chose between gradient-based, adaptive response surface-based, or natural inspired optimization algorithms as well as a mix of them.

Based on well determined laboratory data of the thermal rock properties, which were used as input data and for determining the uncertainty range, a good fit between measurement results and the simulation of the temperature evolution around the heaters could be achieved and, thus, the identification of the thermal in-situ rock properties was successful. Taking the correct simulated temperature evolution as a sound basis for calculating the porewater pressure evolution, a good fit between measurement and simulation results during the heating phases could be achieved as well. The newly implemented constitutive laws that describe the permeability as functions of anisotropic stress and plastic strain have proven their suitability. In general, a material model is available that allows the description of the THM rock behaviour in response to heating for temperatures  $\leq 100^{\circ}$ C.

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# References

ANDRA (2005): Andra research on the geological disposal of high-level long-lived radioactive waste – Dossier 2005 – Results and perspectives, ANDRA, Châtenay-Malabry, France.

DYNARDO (2010): multiPlas – elastoplastic material models for ANSYS, version 6.0. DYNARDO GmbH, Weimar, www.dynardo.de, multiPlas user's manual

DYNARDO (2015): optiSLang- the optimizing Structural Language version 4.2.1, DYNARDO GmbH, Weimar, www.dynardo.de, optiSLang documentation.

Jobmann, M. (2010): Thermophysical properties of drill core samples taken from TED experimental area, Technical Report, Peine, Germany.