

MODELLING INFILTRATION TESTS ON PELLETTIZED BENTONITE UNDER NON-ISOTHERMAL CONDITIONS

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Key words: Infiltration tests, bentonite pellets, thermal effects, coupled THM analysis, nuclear waste

Abstract. A promising alternative to construct engineered barriers for high level nuclear waste repositories is the use of pellets-based material because high dry densities can be achieved with no or minimal compaction effort. It is also planned to subject these materials to temperatures significantly higher than 100°C. The paper reports the results of coupled THM analyses of a heating-hydration test performed on a granular assembly of MX-80 bentonite pellets. The goal is to characterize the material under conditions akin to those of an engineered barrier in a nuclear waste repository. It is shown that the numerical analyses are able to reproduce satisfactorily the observations of the test. This enhances the confidence placed on the computational tool for predicting the behaviour of actual engineered barriers constructed with pellets-based materials.

1 INTRODUCTION

An important component of a significant number of repository designs for deep geological repositories for high level nuclear waste involves the emplacement of an engineered barrier surrounding the canister containing the waste. Expansive clays (bentonite) are adopted as the main material for these barriers because of their low hydraulic conductivity, high retention capacity and its ability to fill and seal irregularities, gaps and fractures. In order to fulfil the safety functions of the engineered barrier, the material has to exhibit a sufficient expansion capacity that it is usually characterized in terms of swelling pressure. Swelling pressure developed during saturation is in turn closely related to the dry density of the material; a minimum value to be achieved during installation is usually specified in the design.

A promising procedure for constructing the barrier involves the use of pellets, i.e. a granular material made of highly compacted bentonite-based granules. Because of the very high density of the pellets, adequate average dry densities may be obtained even with minimal or no compaction effort. Naturally, the properties of this type of material and their dependence on degree of saturation are quite different from conventionally compacted bentonite; it is therefore necessary to conduct a full range of tests to characterize their THM

behaviour and properties. An important component of the testing programme is the performance of column tests in which simultaneous thermal and hydration processes, similar to those expected in an engineered barrier, can be observed under very controlled conditions.

This paper describes the THM analysis of a column test on bentonite pellets performed in the CIEMAT laboratory in Madrid. The main features of the test are presented first followed by a brief description of the numerical formulation used in the analysis. Afterwards, the results of the coupled THM analysis are presented and compared with experimental results.

2 DESCRIPTION OF THE THERMAL COLUMN TEST

The experimental work concerning the column test has been described in detail in [1]. For completeness, some of the main features of the test are given here. The initial state of the sample was as follows: dry density achieved 1.53 g/cm^3 , porosity 0.444, water content 6.4 % and the overall degree of saturation 22%.

The test was performed in a cylindrical cell with an internal diameter of 7 cm and a length of 50 cm. Teflon cell walls are used to limit the amount of lateral heat dissipation. As significant swelling pressures are expected to develop, the cell is covered with steel in order to reduce the lateral expansion of the Teflon walls. A heater is placed at the bottom boundary of the cell whereas hydration is applied from the upper boundary. The thermal condition of the upper boundary is controlled by water circulation at constant temperature. A schematic layout of the test is shown in Figure 1. To provide thermal insulation the cells were laterally surrounded by a layer of dense foam 5-mm thick. Because the lateral heat loss was still considered excessive, the foam was replaced by insulation wool during the running of the test. Temperature and relative humidity were measured at three different elevations along the column (see Figure 1). In addition, heater power and axial stress were also monitored.

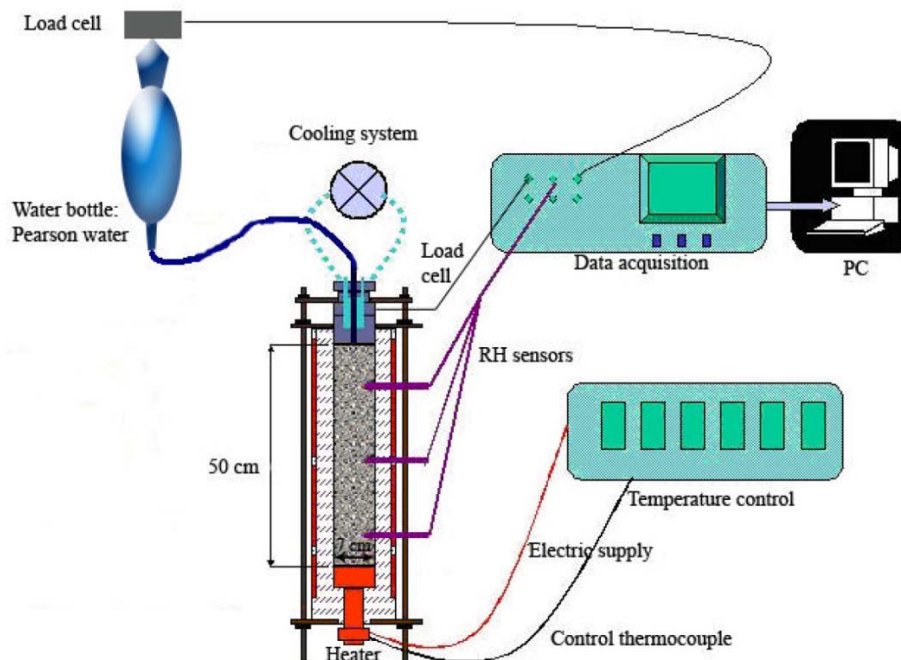


Figure 1: Schematic layout of the column test [1]

The tests were performed in two stages. In the first one, only a thermal gradient was prescribed with no hydration taking place. This stage tries to simulate the early stage of a barrier in a low-permeability argillaceous rock where hydration from the host medium will be minimal. This stage is divided in two parts, in the first one a temperature of 100°C is applied whereas in the second part a temperature of 140°C is prescribed. Afterwards hydration is initiated using a water (Pearson water) with a similar composition to that of Opalinus clay, the host rock in the Mont Terri underground laboratories where a large scale in situ test using the material is being performed.

3 FORMULATION

The THM formulation used is based on the one proposed in [2] applied to clays [3]. The formulation uses a multi-phase, multi-species conceptual model. The porous medium is assumed to be made up of three phases: solid, liquid and gas. Using the compositional approach, the formulation is based on establishing the balance equations for each species: mineral, water and air, instead of using the phases. Thus, the contributions of phase changes automatically cancel. Variables may include a subscript, a superscript or both. The subscript refers to the phase (*s* for solid, *l* for liquid and *g* for gas), whereas the superscript indicates the species (*w* for water and *a* for dry air).

As an example, the balance equation for the mass of water is expressed as:

$$\frac{\partial}{\partial t}(\phi S_l \rho_l w_l^w + \phi S_g \rho_g w_g^w) + \nabla \cdot (\mathbf{j}_l^w + \mathbf{j}_g^w) = f^w \quad (1)$$

where ϕ is the porosity, S_l and S_g the liquid and gas degree of saturation, ρ_l and ρ_g , the liquid and gas densities in Kg/m³ of phase, w_l^w the mass fraction of water in the liquid (close to one in dilute solutions) and w_g^w the mass fraction of water vapour in the gas phase. \mathbf{j}_l^w and \mathbf{j}_g^w are the mass flux of water in the liquid and gas phases respectively. The term f^w is the source/sink term.

Adding the mass balance equations for water and air to the equation for energy balance and momentum balance (equilibrium), the governing equations for the THM problem are obtained. These equations are solved simultaneously at every time step of the analysis. To close the THM formulation it is necessary to specify the relevant constitutive equations that describe the set of phenomena considered. Phase changes (liquid water/vapour and gaseous air/ dissolved air) are assumed to be in equilibrium. The corresponding equilibrium restrictions are also incorporated in the formulation.

4 RESULTS OF THE MODELLING

4.1 Description of the coupled analyses

The calculation axisymmetric geometries included not only the pellets-based bentonite but also the lateral walls and the insulation surrounding the samples on order to achieve a good representation of thermal conditions (Figure 2). A suction value of 123 MPa was adopted for the initial hydraulic state of the bentonite pellets, corresponding to an initial relative humidity value of around 40%. The initial temperature was assumed to be equal to 22.7°C. A 0-flux

condition was applied to the upper boundary of the cells prior to the infiltration phase of the experiment. No vertical displacements were allowed along the upper and lower horizontal boundaries of the bentonite column. The full set of material properties used are given in [4].

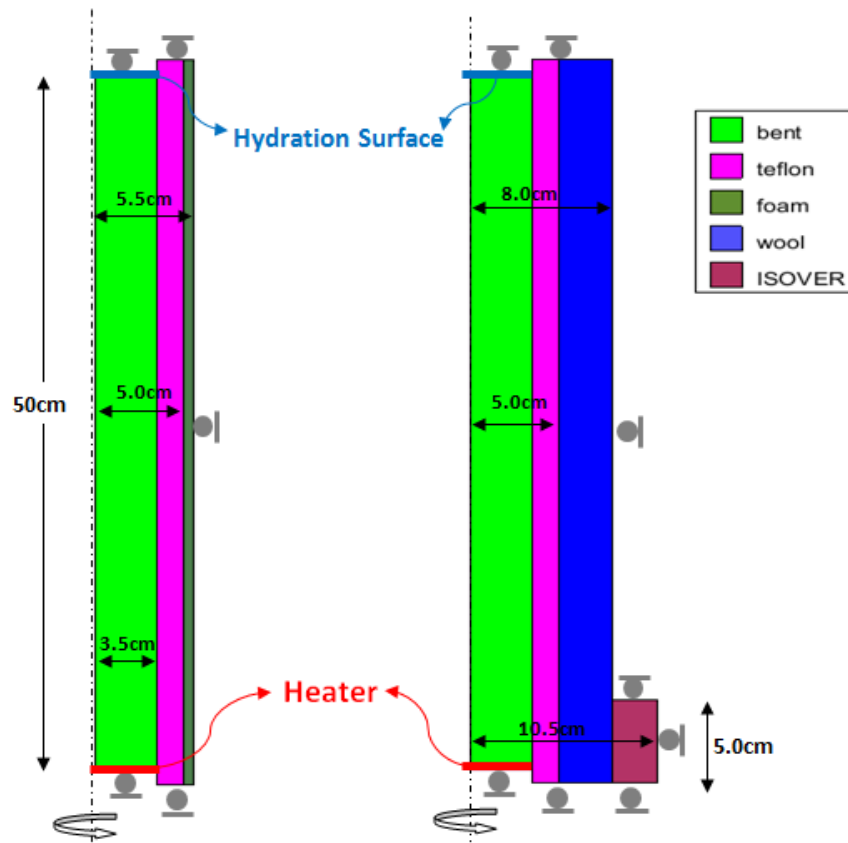


Figure 2: Model geometry and boundary conditions used in the analysis of the column test. a) initial state b) after insulation replacement.

The analyses followed closely the various stages of the real experiments. They involved the following stages:

- Construction of the column cell and emplacement of the isolation material at constant temperature. Initial and boundary conditions prior to the onset of heating were prescribed.
- A first temperature increase at the heater until reaching a target temperature of 100°C. The target temperature was reached 33 minutes after the heater was switched on and temperature was increased linearly. Once the heater temperature was set at 100°C, it was kept constant until the beginning of the second episode of temperature increase.
- Reinforcement of the insulation system. 1518 hours after heating started, the foam initially used was removed and replaced by insulation wool.
- A second temperature increase on the heater surface is applied until reaching a final temperature of 140°C. This heating episode started 3527 hours after the first onset of

heating and the final target temperature was reached in 17 minutes. After that, the temperature on the heater surface was maintained constant until the end.

- Controlled hydration of the bentonite cells. Hydration started 5015 hours after the start of heating. A constant liquid pressure of 0.01 MPa (0.1 bar) was applied to the upper horizontal boundary of the column simulating the hydration process of the cell. This condition has been kept unchanged until the end.

4.2 Results

The computed evolution of temperatures and relative humidity at different locations along the column are plotted in Figures 3 and 4 respectively where they are also compared to the experimental observations. It can be noted that a good agreement is obtained throughout the analysed duration of the test. It is interesting to note the increase of temperatures (both measured and computed) associated with the improvement of isolation. There are some seasonal variations of the temperatures reflecting changes of temperature in the laboratory that have not been introduced in the modelling.

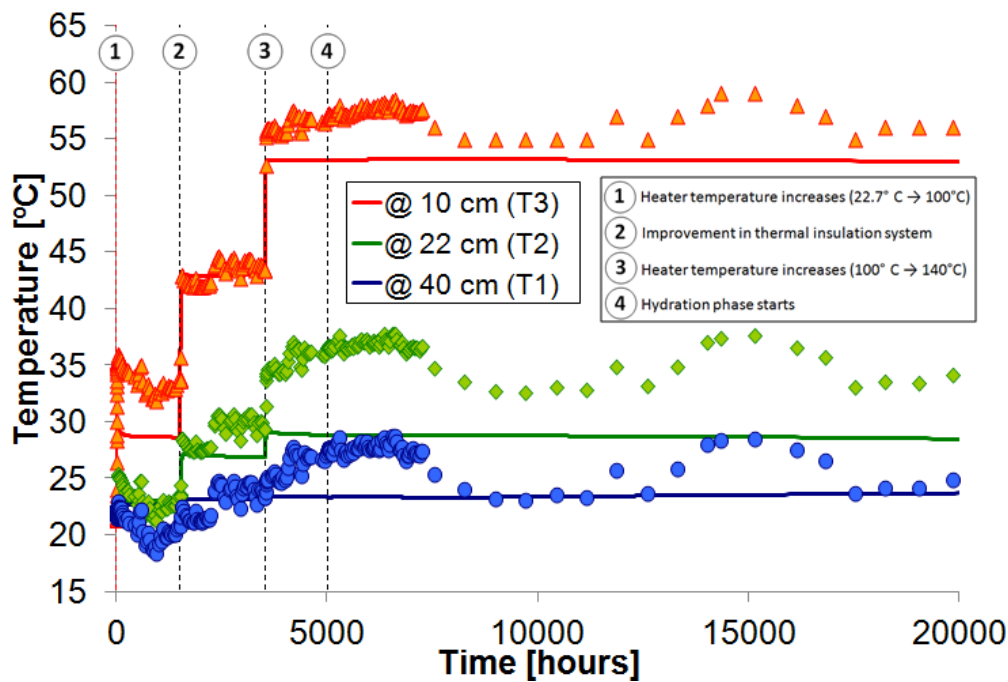


Figure 3: Observed and computed temperatures at different points of the column.

In the thermal stage without hydration, it is apparent that heating brings about water vapour generation at the bottom part of the pellet column (Figure 4). Condensation takes place closer to the top of the bentonite cell where the water vapour (coming from the hot zones by diffusion mechanism) condensates. Vapour condensation leads to an increment of humidity (and consequently, an increase in degree of saturation) in the cooler zones inside the cell as indicated in the RH measurements and model computations for the two sensors further away from the heater. In contrast, after the first RH increase, the degree of saturation decreases near

the heater during the heating experiment as recorded by the sensor RH3. Once hydration starts, relative humidity values tend to increase in all sensors but at different rates, the sensor close to the hydration boundary showing near full saturation. Again the observations are closely tracked by the results of the analysis.

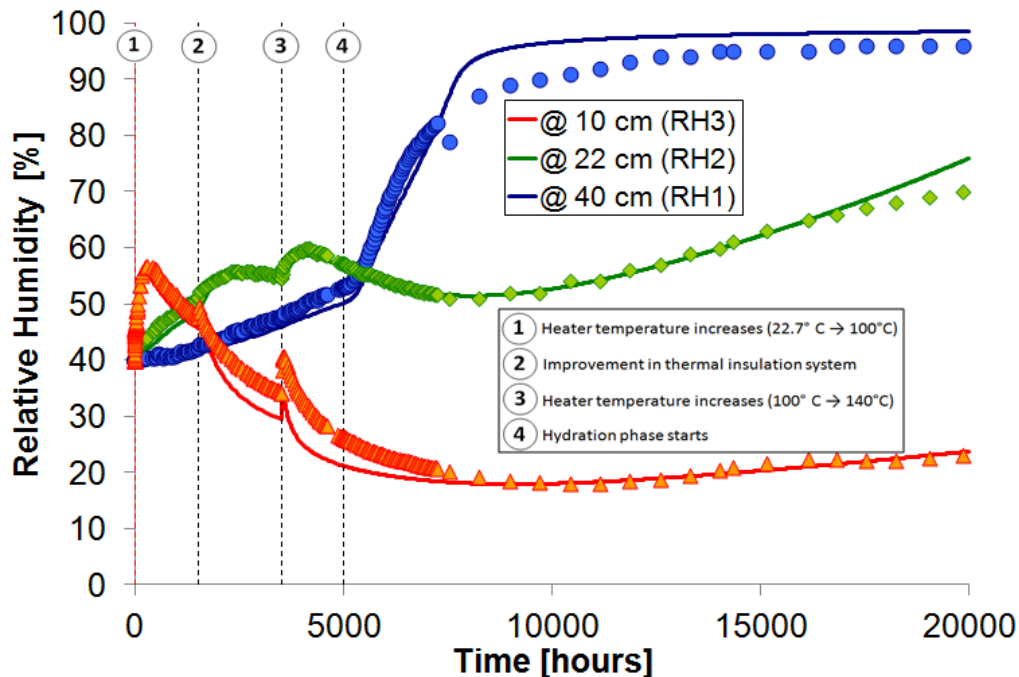


Figure 4: Observed and computed relative humidity at different points of the column.

5 CONCLUSIONS

A column heating-hydration test on a granular assembly of MX-80 bentonite pellets has been simulated using a coupled THM formulation under conditions of temperature reaching up to 140°C. A satisfactory reproduction of the results has been achieved. This enhances the confidence placed on the computational tool for predicting the behaviour of actual engineered barriers constructed with pellets-based materials.

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