Engineering Geology 198 (2015) 94–106

Contents lists available at ScienceDirect

Engineering Geology

journal homepage: www.elsevier.com/locate/enggeo

Numerical modeling of heating and hydration experiments on bentonite pellets

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ARTICLE INFO

Article history:
Received 16 October 2014
Received in revised form 22 September 2015
Accepted 27 September 2015

Keywords:
Radioactive waste disposal
MX-80 bentonite
THM coupling
Multiphase flow
Thermal effect
OpenGeoSys

ABSTRACT

In a common, designed disposal system for high-level radioactive waste, bentonite is used worldwide as a buffer material due to its favorable thermodynamic properties. In-situ experiments at different scales are being conducted in several underground laboratories to investigate the long-term coupled thermo-hydro-mechanical (THM) and chemical behavior of bentonite. Simultaneously, numerous laboratory experiments under well-defined conditions were performed to determine the material properties of bentonite. Since 2012, a laboratory heating and hydration test on MX-80 bentonite has been performed by CIEMAT (*Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas*). The obtained data during the test were analyzed by different research teams within the international DECOVALEX project in order to understand the coupled THM behavior of bentonite and furthermore to determine the thermal-mechanical properties of bentonite. This paper presents a numerical model for fully-coupled THM processes in bentonite based on the finite element method program OpenGeoSys (Kolditz et al., 2012a). In this model, the description of heat conduction is based on Fourier's law, and advection is also considered in the heat transfer. As an important coupling factor from hydraulic process to thermal process, the dependency of thermal conductivity on the water saturation is intensively analyzed. A multiphase flow model considering water evaporation and vapor diffusion is used to describe the hydraulic process. Special attention was also paid on the analysis of the water retention behavior. An elastic constitutive model based on generalized Hook's law was applied to describe the material's mechanical behavior complemented with consideration of the thermally induced strain and the swelling deformation. Good agreement between the calculated and measured data has been achieved concerning temperature, relative humidity, total stress, and water intake. The main coupling processes and bentonite behavior in the experiment could be captured and well analyzed in this model. However, further investigations are also needed, especially for the long-term THM process with respect to water intake.

1. Introduction

MX-80 bentonite is commonly regarded as a buffer material in the disposal of high-level radioactive waste (HLW). As a buffer material, bentonite is filled between canisters and surrounding rock. Thus, the bentonite is expected to experience the maximum temperature in the early post-closure phase (Villar, 2002) in the operation of the nuclear waste repository, which varies between 90° and 150° (Johnson et al., 2002) depending on the repository concepts. Due to high temperatures, de-saturation processes would occur in the near field of canister. Heat transfer would then occur more slowly because of the lower thermal conductivity under the dry state. Furthermore, this drying process could lead to local fracturing due to shrinkage. Afterwards, the buffer material would be re-saturated as a result of groundwater inflow from surrounding rock. During the re-saturation process, the fractures could be sealed due to the swelling behavior.

To demonstrate the feasibility of bentonite as a buffer material in the different repository concepts and to determine the strongly coupled thermo-hydro-mechanical (THM) behaviors in bentonite, many experiments at different scales have been carried out in the underground laboratories. The first, long-term, full-scale experiment was the FEBEX (Full-scale Engineered Barriers EXperiment) experiment in the granitic rock at the Grimsel Test Site in Switzerland (ENRESA, 2000), in which compacted Ca-bentonite was tested under a thermal loading of 100 °C for over 15 years. An extensively coupled THM database is available. A similar database on the MX-80 Na-bentonite was also obtained from the ‘Prototype Repository’ experiment in the Äspö Rock Laboratory in Sweden (Andersson et al., 2005).

MX-80 bentonite is also considered as a buffer material in the repository concept in clay formations. In the Swiss concept for repository of HLW in Opalinus clay, the temperature of the canister surface is estimated at up to 140 °C. A Full-Scale Emplacement (FE) Experiment at Mont Terri underground research laboratory in Switzerland is being

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http://dx.doi.org/10.1016/j.enggeo.2015.09.009

constructed to simulate the long-term coupled THM behavior and to study the interaction between buffer material MX-80 and the saturated Opalinus clay formation under in-situ conditions (Mueller et al., 2012). Additionally, a 1:2 scale heating experiment (HE-E) has been in operation since 2011 in the Mont Terri underground laboratory (Teodori and Gaus, 2011). In site two heaters with the maximum surface temperature of 140 °C (Gaus et al., 2011) were emplaced in a 50-m-long microtunnel of 1.3 m diameter. As buffer material, one section is filled with MX-80 bentonite pellets and the other section is filled with sand/bentonite mixture (65:35) (Fig. 1). Numerous sensors of temperature, pore pressure, humidity and displacement were installed in the boreholes radial and parallel to the microtunnel. A monitoring phase of about 10 years is planned to obtain a long-term database for system understanding.

As complementing to the in-situ experiment, laboratory tests are still necessary to determine the thermal, hydraulic and mechanical properties of clayey materials. However, the great challenge for the measurement of hydromechanical variables under high temperatures lies in the reliability of the experimental techniques, e.g., power interruption, overheating, gas leakage in the system, and heat loss due to insufficient insulation. For the numerical interpretation of long-term experiments, it is important to consider such 'accidents'. In the last two decades, numerous small scale and mock-up scale experiments under well-defined laboratory conditions have been carried out. For example, the FEBEX mock-up test conducted by CIEMAT (*Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas*) (ENRESA, 2000) simulated the long-term Ca-bentonite behavior at a temperature of 100 °C as a comparable experimental setup to the in-situ FEBEX experiment at the Grimsel test site, which is however, under the well-defined boundary conditions and without rock heterogeneity. A series of tests aiming to determine thermo-hydro-mechanical properties of MX-80 used in the Prototype Repository have been conducted by Clay Technology, Sweden (Andersson et al., 2005). Similar experiments for determination of THM properties of the Callovo–Oxfordian claystone from the Bure site (France) have been conducted (Zhang et al., 2010). To complement the HE-E experiment, CIEMAT is performing a long-term laboratory heating and hydration test on MX-80 pellets since 2012. The good dataset is valuable for intensive analysis of the THM behavior and for the determination of the material parameter using numerical methods.

Within the current international cooperative project DECOVALEX (DEvelopment of COupled models and their VALidation against EXperiments) (Hudson and Jing, 2013), one of the tasks is geared toward the understanding of THM processes in bentonite buffers and in argillaceous host rock with the development of numerical models to simulate the HE-E in-situ heating experiment. To validate the numerical model and to estimate the material parameters, the CIEMAT-experiment was carried out. The experiment observations have been analyzed by eight modeling teams using different codes and different numerical methods. The modeling presented in this paper was carried out by the cooperative BGR (Federal Institute for Geosciences and Natural Resources)/ UFZ (Helmholtz Centre for Environmental Research) team, which is based on the OpenGeoSys (OGS) code.

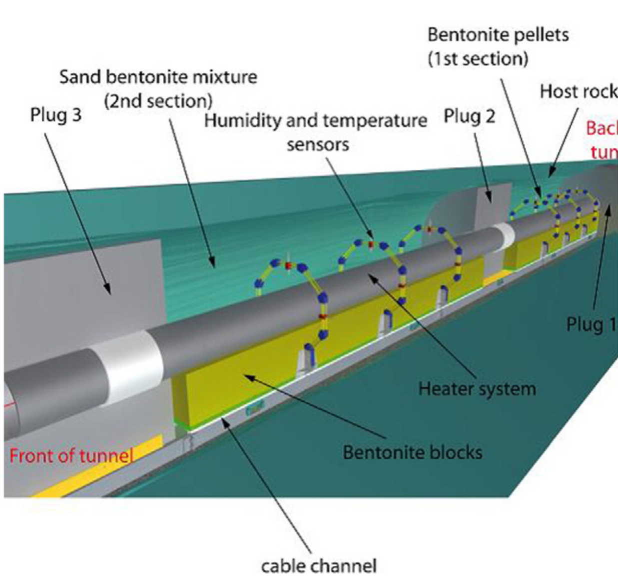

Fig. 1. Lay-out of the HE-E experiment (Teodori and Gaus, 2011).

2. Laboratory experiment

To characterize the material behavior of the MX-80 bentonite pellets and to complement the HE-E in-situ experiment, CIEMAT has been performing since 2012 a long-term laboratory heating and hydration test on MX-80 pellets (Villar, 2012; Villar et al., 2014).

The aim of this laboratory experiment is to estimate the buffer material properties under conditions of fewer uncertainties. The sample was taken from the same material as the buffer used in the HE-E experiment: granular bentonite (sodium bentonite MX-80 from Wyoming, USA) (Plötze and Weber, 2007) and Sand/Bentonite mixture of 65% sand and 35% bentonite. However, in our study only the experiment on MX-80 is simulated.

The MX-80 sample was initially compacted to a dry density of 1.53 g/cm^3. By consideration of the shape and the inner volume of the test cell, a MX-80 column with a diameter of 70 mm and a height of 483.9 mm was fabricated. The initial water content was determined as 6.4% with the initial water saturation degree of 22% and the initial porosity of 0.444 (Table 1).

By the test the MX-80 column is installed inside the cell. The heater is installed in a steel frame (Fig. 2) that has direct contact to the bottom of the sample. To reduce heat losses and for a better heat transfer, the heater is surrounded with Teflon. The cell wall is also assembled with 15 mm of Teflon in order to reduce the lateral heat loss. Additionally, the cell wall is supported by a 4-mm-thick 304 L stainless steel shells in order to avoid the swelling-induced deformation of the sample. In addition to reducing the heat dissipation through the outside wall, the cell is also surrounded by several different insulation materials (Fig. 2). Initially, a 5-mm-thick dense foam was placed around the cell, whose thermal conductivity is 0.04 W/mK. After 1518 h, the insulation system was improved by replacing the dense foam with 30 mm of insulation wool whose thermal conductivity is 0.04 W/mK. Besides, a 25 mm thick ISOVER BT_LV insulation was additionally installed at the bottom of the column with a thermal conductivity of 0.034 W/mK. A porous filter is installed above the top of the sample. With an overhead hydration line, water can be injected from the top into the sample. Three sensors (sensor 1 at 40 cm from the sample bottom, sensor 2 at 22 cm, and sensor 3 at 10 cm, respectively) are placed in the cell in order to record the temperature and humidity evolution. The axial pressure on the top and the water intake are also recorded during the experiment.

During the experiment the sample is subjected initially to heating followed by hydration at constant temperature (Fig. 3) in order to simulate the real heating and re-saturation process in the natural clay barrier of one HLW. The first heating phase lasted from the beginning to

Table 1
Characteristics of the MX-80 pellets (Villar 2012).

Diameter (mm)	70.0
Height (mm)	483.9
Sample mass (g)	3094
Dry density (g/cm^3)	1.53
Void ratio (–)	0.797
Porosity (–)	0.444
Initial water content (%)	6.4
Degree of water saturation (%)	22