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## Design and validation of the THMC China-Mock-Up test on buffer material for HLW disposal



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### ABSTRACT

According to the preliminary concept of the high-level radioactive waste (HLW) repository in China, a large-scale mock-up facility, named China-Mock-Up was constructed in the laboratory of Beijing Research Institute of Uranium Geology (BRIUG). A heater, which simulates a container of radioactive waste, is placed inside the compacted Gaomiaozi (GMZ)-Na-bentonite blocks and pellets. Water inflow through the barrier from its outer surface is used to simulate the intake of groundwater. The numbers of water injection pipes, injection pressure and the insulation layer were determined based on the numerical modeling simulations. The current experimental data of the facility are herein analyzed. The experiment is intended to evaluate the thermo-hydro-mechano-chemical (THMC) processes occurring in the compacted bentonite-buffer during the early stage of HLW disposal and to provide a reliable database for numerical modeling and further investigation of engineered barrier system (EBS), and the design of HLW repository.

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### 1. Introduction

At present, the preliminary repository concept of high-level radioactive waste (HLW) in China is a shaft-tunnel structure, located in saturated zones in granites (CAEA, 2006), as presented in Fig. 1. Repositories are generally designed on the basis of a multiple barrier system concept with engineered and natural barriers between the HLW and the biosphere.

The buffer material, as one of the most important components in the engineered barrier system (EBS), is the last line of defense between waste container and host rock, and will be subjected to high temperature due to heat emitted by the waste and hydration by water coming from the adjacent rocks (Gens et al., 2010). The buffer material is designed to stabilize the repository excavation damaged zone

(EDZ) during tunneling in conjunction of the coupled thermo-hydro-mechano-chemical (THMC) conditions, and to provide low permeability and long-term retardation of contaminant movement (Wang, 2010). A bentonite-based material is often proposed or considered as a possible buffer material for the isolation of the HLW. To guarantee the long-term safety of the engineered barrier, it is necessary to understand the coupled THMC behaviors of bentonite under simulative geological disposal conditions, and subsequently to reveal the property changes of the bentonite over a long period of time.

To understand the complex behaviors of the buffer material located in the coupled THMC environment, in recent years, there has been an increasing interest internationally in the construction of large-scale mock-up experimental facilities in the laboratory and in-situ such as the Long-term Experiment of Buffer Material (LOT) series at the Äspö Hard Rock Laboratory (HRL) in Sweden (Karnland et al., 2000), FEBEX experiment in Spain (Lloret and Villar, 2007), OPHELIE and PRACLAY heater experiments in Belgium (Romero and Li, 2006; Li et al., 2006, 2010), Mock-Up-CZ experiment in Czech Republic (Pacovsky et al., 2007), etc. In these laboratories, very comprehensive knowledge about the disposal of radioactive waste in various geological formations has been accumulated; and adequate techniques for repository construction, waste emplacement in disposal drifts and boreholes, backfilling/sealing of the openings have been developed. The experimental results and achievements obtained from these large-scale experiments provide important references for investigating the behaviors of bentonite under simulative nuclear radioactive waste repository conditions.

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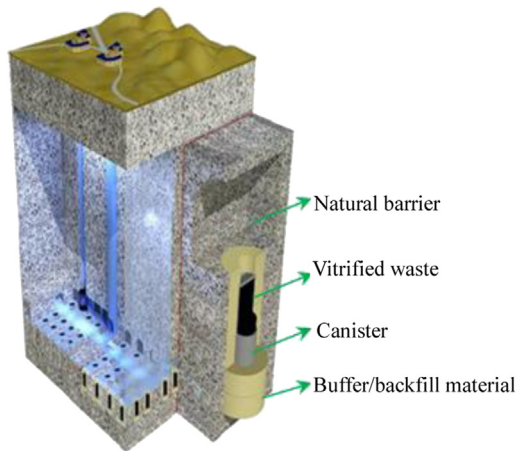


Fig. 1. Preliminary repository concept of HLW in China.

The Gaomiaozi (GMZ) bentonite is considered as the candidate buffer material for the Chinese HLW repository. Lots of basic experimental studies have been conducted and favorable results have been achieved (Liu and Wen, 2003; Liu et al., 2007a; Ye et al., 2009). In order to study the behaviors of the GMZ-Na-bentonite under relevant repository conditions, a large-scale mock-up facility, named as China-Mock-Up, was designed based on a preliminary concept of HLW disposal in China (Liu et al., 2011). The experiment is intended to evaluate the THMC processes in the compacted bentonite-buffer during the early stage of HLW disposal.

The main objectives of the China-Mock-Up include:

- (1) To study the behaviors of GMZ-Na-bentonite under coupled THMC conditions.
- (2) To study the bentonite–canister reaction under coupled THMC conditions.
- (3) To simulate vertical placement of a container with radioactive waste.
- (4) To calibrate the installation method and to verify the validity of sensors.
- (5) To provide a reliable database for numerical modeling and further design of EBS.

The overall approach consists of performing experiments according to the needs for additional studies on key processes during the early EBS evolution. The study will make the most of ongoing experiments being conducted in the laboratory of Beijing Research Institute of Uranium Geology (BRIUG).

## 2. Preparation of the materials

### 2.1. GMZ-bentonite

In this context, the GMZ-Na-bentonite, which has been selected as the most potential buffer material supplier for China's HLW repository, is used. The GMZ-bentonite deposit is located in the northern China, Inner Mongolia Autonomous Region, 300 km northwest of Beijing. The deposit, with bedded ores, was formed in the Late Jurassic. Ore minerals include montmorillonite, coexisting with illite; and gangue minerals include quartz, feldspar, calcite, zeolites, cristobalite, etc. (Wang et al., 2006).

Comprehensive studies have been conducted on the GMZ-Na-bentonite (Chen et al., 2006; Ye and Qian, 2009). The previous studies on GMZ-Na-bentonite show that the bentonite is characterized by high content of montmorillonite (70%) and low impurities. Various experiments have revealed that the GMZ-Na-

bentonite has cation exchange capacity of 77.30 mmol/(100 g), methylene blue exchange capacity of 102 mmol/(100 g), and alkali index of 1.14 (Liu et al., 2007b). The main properties of the bentonite compacted to a dry density of 1800 kg/m<sup>3</sup> are: (a) thermal conductivity of around 1.0 W/(m K) at water content of 8.6%, (b) hydraulic conductivity of  $1 \times 10^{-13}$  m/s, and (c) swelling pressure of 10 MPa (Wen, 2006). Those characteristics indicate that the GMZ-Na-bentonite has very similar properties to those of the mostly investigated MX-80 and FEBEX bentonites.

### 2.2. Material preparation

Compacted bentonite blocks are used as buffer material for HLW disposal. Granular mixtures made of high-density pellets of bentonite are being evaluated as an alternative buffer material for waste isolation (Alonso et al., 2010).

Specially designed steel and a computer-assisted triaxial experiment machine were used to compact the GMZ-Na-bentonite powder into blocks with five different shapes. The square bar-shaped bentonite blocks were subsequently crushed into small pellets in different grain sizes in order to fill the space between the bentonite blocks and the heater/steel tank walls in the China-Mock-Up. The total averaged dry density of compacted bentonite blocks and pellets is 1600 kg/m<sup>3</sup>.

## 3. Design of the China-Mock-Up test

The China-Mock-Up is mainly made up of eight components, namely compacted bentonite blocks, steel tank, heater and corresponding temperature control system, hydration system, sensors, gas measurement and collection system, real-time data acquisition and monitoring system. The compacted bentonite-blocks have been constructed in a large steel tank of 900 mm in internal diameter and 2200 mm in height. The steel tank replaced the host rock to resist the internal pressure that was caused by the pore water pressure and the swelling pressure of the buffer material. An electric heater of 300 mm in diameter and 1600 mm in length, which is made by carbon steel as the substitute of a real HLW container, is placed inside the bentonite-buffer. The EBS is heated by the heater from the ambient temperature to 90 °C. In order to keep the temperature of the buffer material, an insulation layer is placed on the surface of the steel tank.

The groundwater flow is simulated by injecting the formation water (obtained from the host granite rock in the Beishan site, Northwest China) around the outer surface of the buffer material. It can be expected that complex THMC processes will occur in the bentonite-buffer, which will be monitored by a number of sensors installed at various locations in the buffer. The main parameters to be measured in the EBS include temperature, water inflow, relative humidity (suction), swelling and total pressure, metal corrosion, as well as displacement of the heater inside the buffer.

In this study, we will use numerical simulations to design the number of water injection pipes and injection pressure, the insulation layer of China-Mock-Up test. Three groups of numerical simulations on the China-Mock-Up were carried out. Hydro-mechanical (HM) processes simulation was used for the design of the numbers of water injection pipe and injection pressure. Thermo-mechanical (TM) processes simulation was used for the design of the insulation layer. Thermo-hydro-mechanical (THM) processes simulation validated the design.

### 3.1. Constitutive model

In order to reproduce the THM behaviors of the GMZ-Na-bentonite, a coupled THM model is proposed. In this model, the

constitutive law and the main balance equations are used for the numerical simulations.

The modified Cam-Clay model is used to represent the mechanical behaviors under coupled conditions. The model is an incremental hardening/softening elastoplastic model. Its features include a particular form of nonlinear elasticity and a hardening/softening behavior governed by volumetric plastic strain. The failure envelopes are self-similar in shape and correspond to ellipsoids of rotation about the mean stress axis in the principal stress space. The flow rule is associated, and no resistance to tensile mean stress is allowed.

### (1) Yield and potential functions

The yield function corresponding to a particular value  $p_c$  of the consolidation pressure has the form:

$$f(q, p) = q^2 + M^2 p(p - p_c) \quad (1)$$

where  $M$  is a material constant.

The yield condition  $f = 0$  is represented by an ellipse with horizontal axis,  $p_c$ , and vertical axis,  $M$ , in the  $(p, q)$  plane. Note that the ellipse passes through the origin; hence, the material in this model is not able to support an all-around tensile stress. The failure criterion is represented in the principal stress space by an ellipsoid of rotation about the mean stress axis.

### (2) Hardening rule

The size of the yield curve is dependent on the value of the consolidation pressure,  $p_c$ , see Eq. (1). This pressure is a function of the plastic volume change and varies with the specific volume. The consolidation pressure is updated for the step, using

$$p_c^N = p_c [1 + \Delta \epsilon_p^v / (\lambda - \kappa)] \quad (2)$$

where  $\Delta \epsilon_p^v$  is the plastic volumetric strain increment for the step,  $v$  is the current specific volume,  $\lambda$  and  $\kappa$  are material parameters.

### 3.2. Diffusion model

The generalized Darcy's law for multiphase porous medium is adopted to simulate the motion of liquid water:

$$f_w = -\frac{k_{int} k_{r, w}}{\mu_w} (\nabla p_w + g \rho_w \nabla y) \quad (3)$$

where  $p_w$  is the liquid water pressure,  $y$  is the vertical upward directed coordinate,  $g$  is the gravity acceleration,  $\mu_w$  is the dynamic viscosity of the liquid water,  $k_{int}$  is the intrinsic permeability, and  $k_{r, w}$  is the relative permeability.

Based on the law of conservation of energy, the balance equation is defined as

$$\frac{\partial Q}{\partial x} = \frac{\partial}{\partial x} \left( \lambda \frac{\partial T}{\partial x} \right) \quad (4)$$

where  $T$  is the temperature ( $^{\circ}\text{C}$ ),  $Q$  is the heat generated by the canister,  $x$  is the thermal transfer directed coordinate, and the origin is located at the surface of the canister.

The heat generated by the canister is equal to the heat absorbed by the bentonite blocks, thus the equation can be defined as

$$C\gamma \frac{\partial T}{\partial x} = \frac{\partial}{\partial x} \left( \lambda \frac{\partial T}{\partial x} \right) \quad (5)$$

where  $\gamma$  is the thermal conductivity of bentonite, and  $C$  is the specific heat of the bentonite.

The heat transfer is assumed to follow the Fick's diffusion law; accordingly, the heat transfer between the bentonite blocks is defined as follows:

$$\Phi(x) = -k \frac{\partial T}{\partial x} \quad (6)$$

where  $\Phi(x)$  is the heat transfer flux, and  $k$  is the heat exchange coefficient.

### 3.3. Material parameters and approach

The material parameters used in the model are determined by the experimental results conducted by Liu et al. (2007a). The THM parameters are based on the work of basic experiments, including mechanical property, hydraulic conductivity and thermal conductivity.

Some material parameters used in the model are shown in Table 1. In this study, FLAC<sup>3D</sup>, a three-dimensional (3D) explicit finite difference code, was used. It is a commercial code provided by Itasca Consulting Group and widely used in various civil and mining engineering projects. FLAC<sup>3D</sup> also contains a powerful built-in programming language, FISH, allowing users to define new variables and functions. The stereo-diagram of the model is presented in Fig. 2.

### 3.4. Hydro-mechanical processes simulation

Table 2 shows the results of numerical simulation of coupled HM processes. We can see that the saturation time of bentonite in the China-Mock-Up decreased from 12 years to 5 years with the increase in numbers of water tubes at injection pressure 2 MPa (Fig. 3). Fig. 4 shows the curve of saturation time with water pressure. The saturation time decreased with the increase of water pressure. In other words, the numbers of water tubes in conjunction with injection pressure have significant effects on the saturation time of bentonite.

The development of stresses is induced by the swelling pressure of the compacted bentonite, as a result of the resaturation. The stress concentration occurs in the middle and the corner of the steel tank in Fig. 5.

### 3.5. Thermo-mechanical processes simulation

Results of numerical simulations of coupled TM processes are shown in Fig. 5. The development of stresses induced by thermal expansion may induce stresses due to the confinement of the bentonite by the steel tank. The stress concentration is observed in the middle and the corner of the steel tank. By comparing the two temperature contours of Fig. 6, we can see that the ambient temperature has an effect on the thermal distribution of the China-Mock-Up. Thereby, an insulation layer was covered around the China-Mock-Up in order to reduce the effect of the ambient temperature.

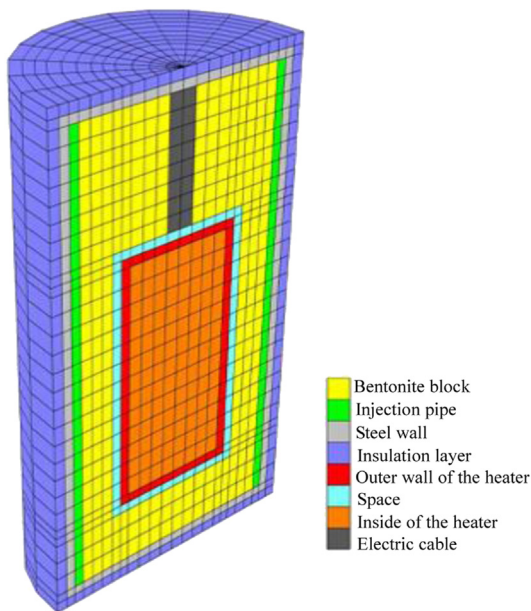
### 3.6. Thermo-hydro-mechanical processes simulation

Taking into account heat, water flow, swelling pressure and permeability of buffer material, the evolutions of temperature, saturation, and stress in the buffer material under THM coupling conditions were analyzed.

Comparing the TM and THM simulations, it is found that the H (hydration) has a minor effect on the temperature distribution.

**Table 1**  
Material parameters used in the model.

Material	Dry density (kg/m <sup>3</sup> )	Bulk modulus (Pa)	Shear modulus (Pa)	Porosity (%)	Coefficient of permeability (m/s)	Thermal conductivity (W/(m K))	Specific heat (J/(kg K))	Linear expansion coefficient	Poisson's ratio
Steel wall	7800	$1.46 \times 10^{11}$	$8.33 \times 10^{10}$	0.1	$1.0 \times 10^{-15}$	48	460	$1.0 \times 10^{-5}$	0.26
Bentonite block	1800	$1.29 \times 10^9$	$3.06 \times 10^8$	10	$1.3 \times 10^{-13}$	0.892	175	$3.0 \times 10^{-6}$	0.39
Insulation layer	100	—	—	—	—	0.04	—	—	—



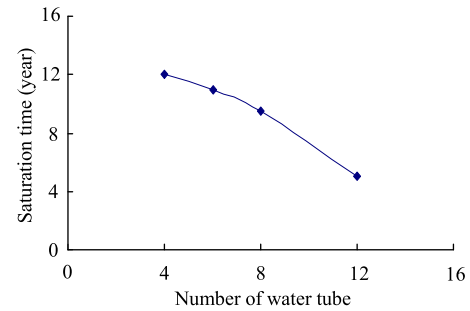
**Fig. 2.** Stereogram of the model (longitudinal view).

Note that the thermal conductivity can be induced by changes in saturation variations. Because of the lower permeability of the compacted bentonite, it will need more than 10 years to saturate the compacted bentonite in the China-Mock-Up, and the drying effect is dominant at the beginning of the operation of HLW repository. The thermal gradient induced by the waste-released heat causes, first, a de-saturation in the zone close to the heater, followed by a resaturation.

The contours of saturation at 1, 3 and 10 years in the THM cases are displayed in Fig. 7. The development of stresses is varied due to different mechanisms: first, thermal expansion may induce stresses because bentonite is confined by the steel tank; then, the swelling pressure of the compacted bentonite is resultant from resaturation. Thermal expansion induced stresses are extremely important in the buffer during the beginning stage, thus the swelling pressure induced stresses play an extremely important role in the long-term behavior of buffer. The stress concentration basically occurs in the middle and the corner of the steel tank.

**Table 2**  
Results of numerical simulations of coupled hydro-mechanical processes.

Number of water tube	Injection pressure (MPa)	Saturation time of bentonite (year)
4	2	12
6	2	11
6	3	10
6	4	8
8	2	9–10
8	4	7–8
8	5	6
12	2	5



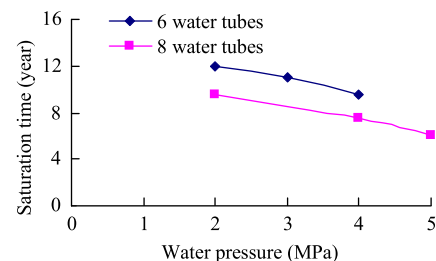
**Fig. 3.** Curve of saturation time with the number of water tubes at the water pressure 2 MPa.

## 4. Validation of the China-Mock-Up

### 4.1. Test procedure

The China-Mock-Up experiment was assembled completely on 10 September 2010. The real-time data acquisition and monitoring system has recorded all data from 1 April 2011. The heater was switched on to reach a low temperature of 30 °C from 1 April 2011 until 8 July 2011. The THMC experiment was commenced on 8 July 2011. The power rose at 1 °C/d to reach a maximum temperature of 90 °C and this temperature was then kept constant. The hydration process was carried out using the Beishan groundwater as shown in Table 3. The initial injection pressure was 0.5 MPa, and the injection rate was 400 g/d. The injection rate was raised to 600 g/d after 300 days, and then to 1200 g/d gradually. The total injected water volume was 104,662 g on 12 July 2012.

The China-Mock-up is equipped with 4 water tubes and 10 different types of sensors to monitor the performances of GMZ-Na-bentonite under coupled THMC conditions. The 6 sensor types inside the China-Mock-Up include stress sensor, hydraulic pressure sensor, LVDT displacement sensor, temperature sensor, relative humidity (RH) sensor and electrochemical corrosion sensor. Except the temperature sensor and the RH sensor, the other 4 sensor types consisting of Coriolis mass flow meter, fiber Bragg grating (FBG) strain/temperature sensor, resistance strain gauge and dial gauge are located outside the mock-up. The sensors placed in the bentonite have provided reasonable and consistent recordings. The time variations associated with the temperature, RH, and stress of the compacted bentonite are analyzed in this paper.



**Fig. 4.** Curves of saturation time with water pressure.



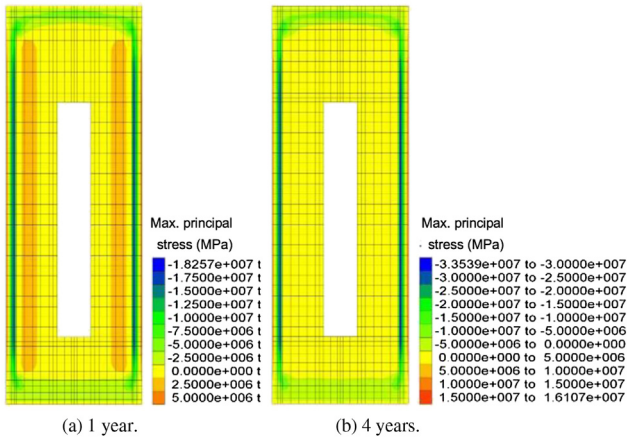


Fig. 5. The maximum principal stress contours at 1 and 4 years.

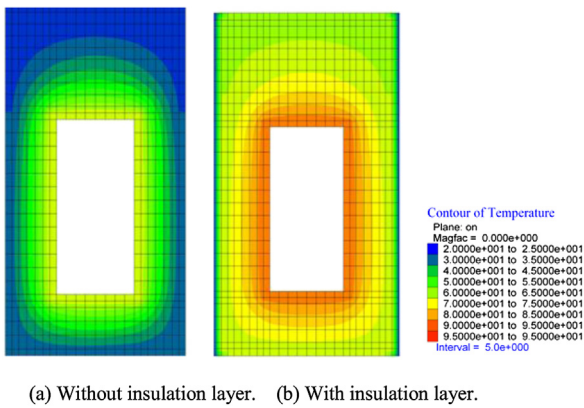


Fig. 6. Temperature contours of coupled thermo-mechanical processes (temperature reached thermal equilibrium).

4.2. Temperature distribution

The distribution of temperature in the China-Mock-Up is illustrated in Fig. 8. It is inhomogeneous in vertical direction and much higher in the central part. The temperature at the top of the heater is higher than that at the bottom because of heat transfer and hydration of gravity. The temperature distribution is influenced by the thermal conductivity and the specific heat of the bentonite. It is strongly related to the degree of saturation because the thermal conductivity of bentonite increased with the increase of degree of saturation.

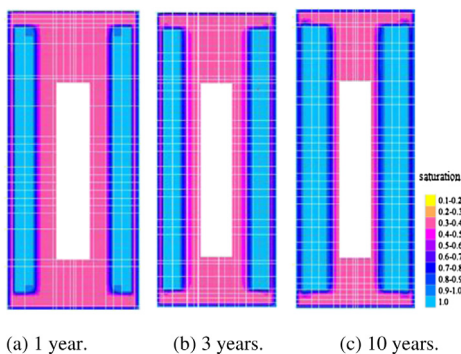


Fig. 7. Saturation contours of the China-Mock-Up.

Table 3  
Chemical compositions of groundwater from Beishan (unit: mg/L).

Chemical compositions										
F <sup>-</sup>	Cl <sup>-</sup>	NO <sub>3</sub> <sup>-</sup>	SO <sub>4</sub> <sup>2-</sup>	CO <sub>3</sub> <sup>2-</sup>	HCO <sub>3</sub> <sup>-</sup>	Na <sup>+</sup>	K <sup>+</sup>	Mg <sup>2+</sup>	Ca <sup>2+</sup>	
4.18	771	8.64	718	92.3	0.6	798	4.8	31.4	177	

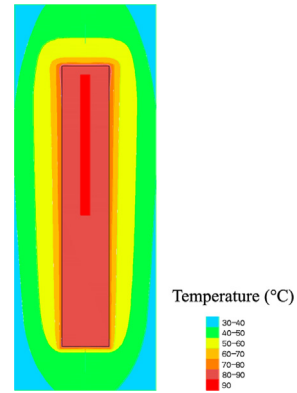


Fig. 8. Temperature distribution in the China-Mock-Up.

4.3. Relative humidity distribution

The RH distribution in the China-Mock-Up is illustrated in Fig. 9. The RH variations are observed to be strongly influenced by the competitive mechanisms such as the saturation process induced by the water penetration and the drying effect by the heater, as well as the gravity. The RH near the heater is lower than the place in vicinity of the water tubes. Water supply is first concentrated on the bottom of the vertical tank. With the saturation of bentonite pellets near the water tubes and due to the extremely low permeability of compacted bentonite, the water supply is then gradually going to the top of the vertical tank. Accordingly, the RH near the bottom is higher than that at the top.

4.4. Stress distribution

The stress sensors were put in three directions in the bentonite blocks and pellets (Fig. 10). The stress evolution in the compacted bentonite may be influenced by several mechanisms, including the gravity, the thermal expansion induced by high temperature, and the swelling pressure generated by water penetration. In Fig. 11, the stresses recorded by the sensors in different directions are given. The stress is higher at the bottom of heater due to the gravity of

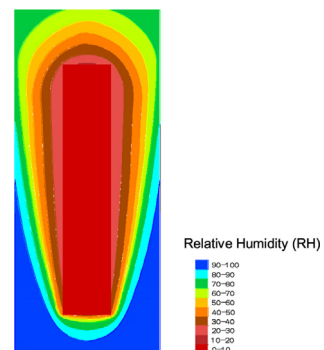


Fig. 9. The relative humidity distribution in the China-Mock-Up.

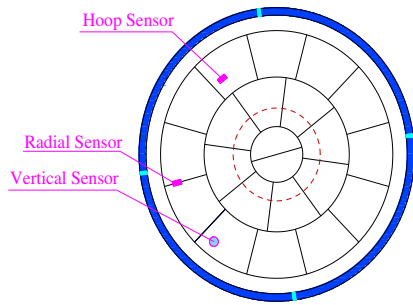


Fig. 10. Stress sensors in the compacted bentonite.

heater and water. Because the mass of the heater is 1000 kg, the pressure under the heater by its weight is 1.24 MPa. The stress around the heater is lower which could be attributed to the stress release induced by the initial gaps between the bentonite blocks and pellets with heater and steel tank, and also the gaps between the sensors and blocks.

4.5. Comparisons between simulation and experimental results

A two-dimensional (2D) axisymmetric finite element simulation is performed. The heating is modeled by imposing the temperature on the nodes of the sample in contact with the heater. The hydration procedure is modeled by increasing the water pressure applied on the nodes of outer boundary. The steel tank is supposed to be impermeable to the water flows. The system is initially set at a temperature of 20 °C, and the gas pressure is supposed to be fixed at the atmospheric pressure. The compacted bentonite has an initial water saturation of 48% and a void ratio of 0.57.

Fig. 12 shows the temperature evolution in the lateral direction. It can be noticed that the calculated temperatures are a little higher than the experimental ones. The reason is that there is an installation space of 5 cm between the heater and the compacted bentonite and also between the compacted bentonite. All these phenomena lead to the low thermal conductivity but they are not considered in the model.

The evolution of RH over elapsed time at point A with coordinates  $r = 0.3$  m and  $z = 0.123$  m is illustrated in Fig. 13. It is noticeable that the numerical results are slightly lower than the experimental ones at the analyzed point A. This can also be attributed to the existing gaps. The gaps between the bentonite blocks or between the blocks and the pellets will lead to form preferential pathways for the migration of water. The injected

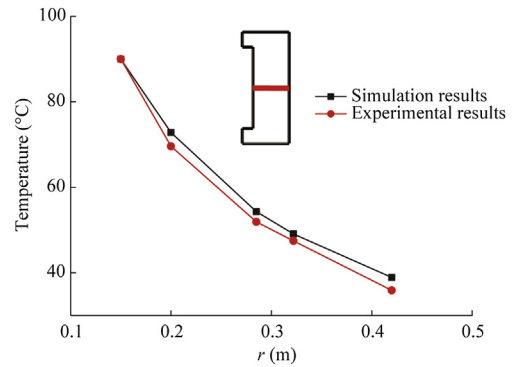


Fig. 12. The temperature comparisons between simulation and experiment, in the middle of China-Mock-Up (after 1 year).

water penetrates into the bentonite along the gaps between the bentonite blocks and pellets, and also along the cable of the sensors.

The swelling pressure evolution at point B with coordinates  $r = 0.15$  m and  $z = 0.123$  m is depicted in Fig. 14. It can be noted that the simulation results are a little higher than the experimental ones. This can be attributed to two reasons: the fact that the bentonite has a very low permeability can make the arrival of water to the inner parts very slow, suggesting that the saturation process of whole barriers is not finished yet; stress release induced by the initial gaps between the bentonite blocks and pellets, and also the gaps between the swelling pressure sensors and the blocks could be another reason.

5. Conclusions

The China-Mock-Up as a large-scale mock-up facility, based on a preliminary concept of HLW repository in China, has been designed, constructed and operated in the laboratory of BRIUG. The experiment facility has worked well for more than 500 days. A lot of valuable data about the evolutions of compacted bentonite and experience about how to evaluate the suitability of buffer material under long-term THMC coupled condition have been obtained for the first time.

The saturation time of compacted bentonite decreased with the increase of numbers of water tubes and water pressure. An insulation layer around the China-Mock-Up played an important role in reducing the effect of the ambient temperature.

The temperature distribution is influenced by the thermal conductivity which is increased with the increase of degree of saturation and the specific heat of bentonite. The RH variation is found to be strongly influenced by the competitive mechanisms such as the saturation process induced by the water penetration

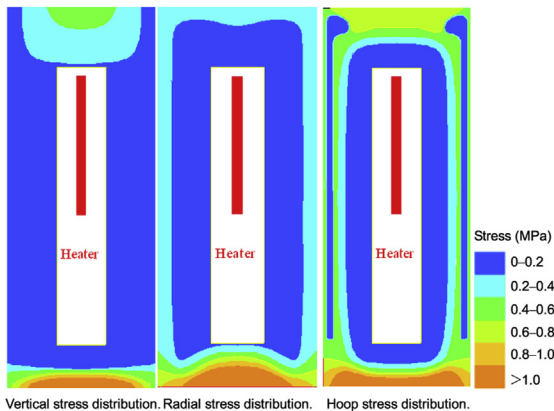


Fig. 11. Stress distribution in the China-Mock-Up.

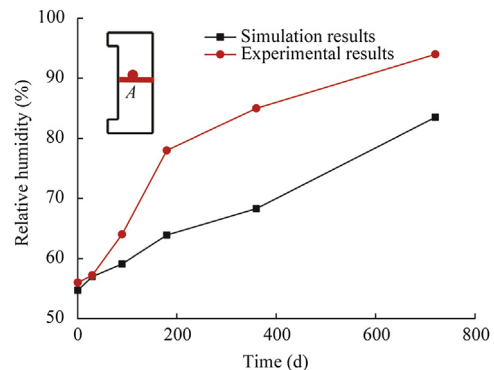
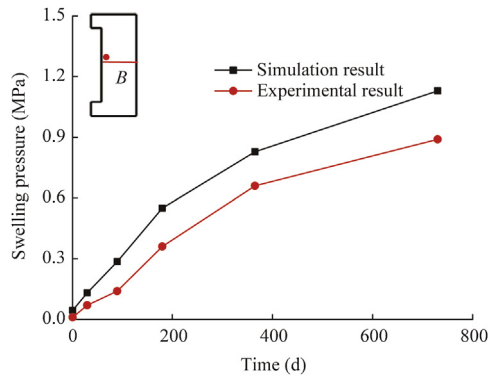


Fig. 13. The relative humidity comparisons between simulation and experiment at point A.



**Fig. 14.** The swelling pressure comparisons between simulation and experiment at point B.

and the drying effect by the heater, as well as the gravity. The stress evolution in the compacted bentonite may be influenced by the gravity, the thermal expansion induced by high temperature, and the swelling pressure generated by water penetration.

With the determined parameters and proposed model, the numerical simulations are accordingly carried out. Based on the comparisons between the numerical results and experimental results, it is suggested that the coupled THM phenomena of GMZ bentonite can be well reproduced by the proposed model.

The parameters and evaluation of THMC processes in the compacted bentonite-buffer during the early phase of HLW disposal can provide a reliable database for numerical modeling and further investigations of EBS, and the design of HLW repository.

### Conflict of interest

We wish to confirm that there are no known conflicts of interest associated with this publication and there has been no significant financial support for this work that could have influenced its outcome.

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