Thermo-hydraulic-mechanical coupling analysis on a heating test in unsaturated ground

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ABSTRACT: In relating to the feasibility of geological disposal of high-level nuclear waste, numerous experimental investigations and numerical simulations have been conducted to guarantee the safety and the efficiency of the geologic sealing structure in long time period. Thermo-hydraulic-mechanical coupling (THM) problem is considered as one of the most important factors in evaluating the whole process of the geological disposal of the nuclear waste. In this paper, a heating experiment (Munoz, 2006) has been simulated to investigate the THM problem in the unsaturated ground, using a program of finite element method (FEM) named as SOFT. The program is based on the finite element-finite difference scheme (FE-FD) in fully coupled soil-water-air three-phase field theory under non-isothermal condition. In the simulation, a rational constitutive model, that takes a Bishop-type skeleton stress and the degree of saturation as the state variables, is adopted. The model can describe the behavior of saturated and unsaturated soil automatically. According to the simulation results, it is known that the present simulation can properly describe the THM behaviors observed in the heating experiment such as the hydration of water, the evolution of temperature, the evolution of pore water pressure to some extent.

INTRODUCTION

Governing Equations

As the consequence of using radioactive materials in industrial, medical, military, a great challenge has been faced for the disposal of radioactive waste, especially for high-level radioactive waste (HLW). Until now, deep geologic disposal is considered as a valid and feasible way based on the concept of isolation from the biosphere, in which a nuclear waste repository is usually excavated below 300m within a stable geologic environment. It usually consists of three barriers: natural barrier, engineered barrier and technological barrier as shown in Fig.1. The technological barrier is a temporary canister including vitrified HLW during the transportation and storage. Engineered barrier is usually consisted of buffer material. Unsaturated bentonite is

foreseen in many countries as the best candidate for buffer material because of its low hydraulic permeability, micro-porous structure, good sorption properties and swelling capacity. Natural barrier is usually soft rock or clay with low permeability.



FIG.1. Multiple barrier concepts in deep geologic disposal

The engineered barrier and natural barrier will be subjected to high temperature released from the HLW, which will give rise to the coupled THM problem. In addition, the bentonite is usually unsaturated during initial period, and will therefore be subjected to hydration from the surrounding rock, triggering further complex coupled THM phenomena. In order to have a good understanding of the processes that occurs in the near field, many larger-scale heating experiments in underground laboratories had been done around the world, e.g., the works by Gens et al. (2007, 2009), Munoz (2006). In reality, however, the heating period caused by the high-level nuclear waste disposal will last for tens of thousands years or even longer for some radioactive substances. Therefore, sometimes it is impossible to reproduce the whole process in the field tests. Numerical simulation will be another effective method to describe and predict the above-mentioned THM behaviors on the condition that the numerical method is able to fit the results of field experiments, at least in a limited period.

The purpose of this paper is to understand and explain unsaturated water flow, temperature and mechanical behavior of the geomaterials during the hydration, heating and cooling phase. Two-dimensional (2D) finite element analysis of a field heating experiment (Munoz, 2006) is conducted using a program named as SOFT. In this research, thermo-mechanical behaviors of the ground are described by the unsaturated model proposed by Zhang and Ikariya (2011). By comparing the numerical results with the test results, the applicability of the proposed numerical method is verified.

BASIC THEORIES OF THM MODELLING

Governing Equations

For simplicity, the phase change due to the increase of temperature emitting from the nuclear waste is not considered in the proposed program. The governing equations of soil-water-air three-phase coupling problem under non-isothermal condition can be classified into four groups: equilibrium equation, continuity equation of water, continuity equation of air and energy equation.

I. Equilibrium equation

$$\frac{\partial \sigma_{ij}}{\partial x_i} + \rho b_i = 0 \tag{1}$$

II. Continuity equation for water phase

$$\frac{\dot{\varepsilon}_{ii}^{s}}{n} - \frac{k^{w}}{\gamma^{w}} \frac{\partial^{2} p^{w}}{\partial x_{i} \partial x_{i}} - \frac{1}{K^{w}} \dot{p}^{w} + \frac{\dot{S}_{r}}{S_{r}} = 0$$
⁽²⁾

III. Continuity equation of air phase

$$\frac{\dot{\varepsilon}_{ii}^{s}}{n} - \frac{k^{a}}{\gamma^{a}} \frac{\partial^{2} p^{a}}{\partial x_{i} \partial x_{i}} - \frac{1}{K^{a}} \dot{p}^{a} - \frac{\dot{S}_{r}}{1 - S_{r}} = 0$$
(3)

IIII. Energy equation

$$\rho c \frac{\partial T}{\partial t} = k_t \frac{\partial^2 T}{\partial x_t \partial x_i} + Q \tag{4}$$

where b_i is the body force, σ_{ij} and ε_{ij} are the total stress tensor and the strain tensor. S_r is the degree of saturation; K is the bulk modulus, k (k_w , k_a) is the permeability of water or air; n is the porosity of soil. c and k_t are the mean specific heat of soil and mean heat conductivity of soil. T and Q are temperature and heat source. In the equations, the superscript of s, w and a denote the solid, water and air phases respectively.

Constitutive Model

The proposed program is based on a simple elastoplastic constitutive model for unsaturated soil proposed by Zhang and Ikariya (2011) in which the Bishop-type skeleton stress and the degree of saturation is used as the state variables. The constitutive model is able to describe not only the behavior of the unsaturated soil but also the saturated soil because the skeleton stress can smoothly shift to effective stress if the saturation changes from an unsaturated state to a saturated state. In the model, a simple moisture characteristics curve (MCC) considering wetting-drying moisture hysteresis of an unsaturated soil is also proposed. Meanwhile the overconsolidation or the density of soil is also properly described based on the concept of subloading (Hashiguchi and Ueno, 1977). The main feature of the model is that the model can describe both the saturated and the unsaturated state of a soil in a unified way using one set of parameters. A detailed description of the constitutive model and the MCC can be referred to the work (Zhang and Ikariya, 2011).

NUMERICAL SIMULATION OF HEATING EXPERIMENT

Brief Description of Heating Experiment

The heating experiment is a large-scale heating test carried out in the Mont Terri Underground Rock Laboratory (Munoz, 2006). The objectives of the heating experiment were to acquire knowledge about the coupled THM processes in the host rock and bentonite buffer.



FIG.2. 3D view of the Mont Terri Underground Rock Laboratory and the location of the HE niche (Munoz, 2006)





The site of the heating experiment was located on the so-called "HE niche" on the west wall of the New Gallery of the underground rock laboratory, in the shaly faices of the Opalinus clay formations. Fig.2 shows the 3D view of the Mont Terri Underground

Rock Laboratory and the location of the HE niche.

A vertical borehole 300mm in diameter and 7.0m in depth, identified as BHE-0, was drilled in the niche floor as shown in Fig.3. A heating tube with an external diameter of 100mm was placed in the axis of the borehole BHE-0. A heater of 75mm in diameter and 2.0m in length was placed into the heating tube. Details of the setup of the test are shown in Fig.4.

The heating experiment was conducted in 3 different phases. The first phase consists of the hydration of the bentonite buffer, which lasted 982 days. The hydration of the bentonite buffer was performed at four different depths at piezometric head of 2.0 m over the niche floor and the surrounding natural rock. The second phase is heating phase once the bentonite buffer was fully saturated. Firstly, heat power was applied in steps of 140W, 150W, 285W and 580W, until the heat-buffer contact reached a temperature of 100 °C. Then, a constant temperature of 100 °C was maintained at the heater-bentonite contact, with a heating period of 540 days. Finally the heat power was switched off and the cooling phase began. In the experiment, the pore water pressure and the temperatures at some selected points are measured.

Numerical simulation and results

Due to the symmetry condition, only half of the area is considered. Fig.5 shows the 2D FEM mesh and mechanical boundary condition. In the analysis, the calculated results of THM variables at some positions, marked with orange line in Fig.5, are selected to compare with the test results. For simplicity, the materials are assumed to be homogeneous and isotropic, focusing on THM coupling process in the rock-buffer system. An isotropic stress state with a magnitude of 5MPa is assumed in the simulation, the same as the assumption in the wok by Munoz (2006). A total water head of 40m is given for the host rock, and initial temperature is 15 °C, the same as the field conditions. The atmospheric air pressure is kept constant. Material parameters



 Table 1 Material parameters of bentonite and rock

of the bentonite and the rock used in the simulation are listed in Table 1.

Fig.6 shows the MCC of the bentonite and the host rock used in the simulation. It is found that the calculated MCC of the bentonite and the host rock can well describe the test results. The parameters of the MCC of the bentonite and the host rock are listed in Table 2.In the simulation, the initial degree of saturation of the bentonite buffer is 70%, which corresponds to a suction of s=136 MPa, measured at the field test.

It is well known that the permeability of water is dependent on the degree of saturation, that is, the permeability increases along with the increase of the saturation. The permeability of water, however, was not measured in the test. In the THM analysis on the heating test, as an alternative, an interpolation method employing some values of the permeability at some specified saturation is used to simulate the change of the permeability with saturation. The relation between the permeability of water and the degree of saturation used in the analysis is shown in Fig.7 in order to fit the results of heating experiment.



FIG.6. Moisture characteristic curve of bentonite and host rock



FIG.7. Estimated relationship between permeability of water and degree of saturation

	bentonite	rock
Saturated degrees of saturation S_r^s	1.00	1.00
Residual degrees of saturation S_r^r	0.40	0.40
Parameter corresponding to drying AEV (kPa) S_d	11000	21000
Parameter corresponding to wetting AEV (kPa) S_w	800	1000
Initial stiffness of scanning curve (kPa) k_{sp}^{e}	25000	90000
Parameter of shape function c_1	0.000001	0.00003
Parameter of shape function c_2	0.000005	0.00006
Parameter of shape function c_3	30.0	50.0

Table 2 Material parameters of Shirasu



FIG.8. Change of degree of saturation for bentonite during hydration phase



FIG.9. Change of degree of saturation for rock during hydration phase

Fig.8 shows the time evolution of the degree of saturation at different positions with time. It is known from the figure that the required time to fully saturate the bentonite is 400 days approximately. In the figure, D is the distance away from the heater

Fig.9 shows the transitory process of the degree of saturation in the surrounding rock at different positions with time, in which de-saturation and re-saturation process were clearly observed. It is found from the figure that the rock reaches the full saturation again after approximately 600 days of the hydration.



FIG.10. Distribution of the degree of saturation at some specified times during hydration phase

Fig.10 shows the distribution of the degree of saturation at specified time during the hydration phase. It is found that the rock near the bentonite firstly changes from saturated state to unsaturated state, this is because the water cannot transport in time due to the low permeability of rock. Later the rock was re-saturated with the migration of pore water.



FIG.11. Change of temperature with time at different positions in heating phase

Fig.11 shows the evolutions of temperatures at different positions away from the heater. It is known that the THM analysis can also well describe the change of temperatures measured in the HE-D experiment on the whole, such as the sharp increase and the sharp decrease of the temperature for all selected positions.



FIG.12. Temperature distributions at different time during heating phase



FIG.13. Change of excessive pore water pressure with time at different positions during heating and cooling phases

Fig.12 shows the comparison between the calculated and measured temperature distributions at different times along a cross section. It is known from the figure that the nearer the distance from the heater is, the higher the temperature will be. There is no prominent increase of temperature at the distance 5m away from the heater due to the low thermal conductivity of the rock.

Fig.13 shows the change of excessive pore water pressure with time at different positions during heating and cooling phases. It is known from the figure that the increase of temperature generates a significant increase of positive excessive water

pressure, and the decrease of temperature will give rise to a decrease of the excessive water pressure. The change of the excessive pore water pressure is mainly due to the fact that thermal expansion coefficient of water is much higher than that of the rock. Owing to the low permeability of rock, the drainage is slow and therefore the expansion of the pore water is impeded, resulting in an increase of the pore pressure at the initial time of heating. Later, as the migration of the pore water, the excessive pore water pressure is allowed to dissipate and consequentially turns to decrease. The simulation can well describe the observed behavior on the whole.

CONCLUSIONS

In this paper, a heating experiment (Munoz, 2006) is simulated, using a program of finite element method (FEM) named as SOFT, in order to investigate the THM behavior of bentonite-host rock composite structure under unsaturated condition. The program is based on a FE-FD scheme in fully coupled soil-water-air three-phase field theory under non-isothermal condition. In the simulation, a rational constitutive model using the Bishop-type skeleton stress and the degree of saturation as the state variables is adopted, which can describe the behavior of saturated and unsaturated soil in unified way. Based on the simulated results, it is known that the present simulation can properly describe the THM behaviors observed in the heating experiment such as the hydration of water, the evolution of temperature, the evolution of excessive pore water pressure to some extent. It is, therefore, possible to apply this numerical method to investigate the real field problem in the geologic disposal of high-level radioactive waste (HLW).

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