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THM coupling sensitivity analysis in geological nuclear waste storage

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ABSTRACT

A deep geological repository involving a multi-barrier system constitutes one of the most promising options to isolate high-level radioactive waste from the human environment. In order to certify the efficiency of waste isolation, it is essential to understand the behaviour of the confining geomaterials under a variety of environmental conditions. The efficiency of an Engineered Barrier System (EBS) is largely based on thecomplex behaviour of bentonite. To contribute to a better understanding of the processes involved in the EBS, a case study for sensitivity analysis has been defined and is studied using a thermo-hydro-mechanical (THM) finite element approach including a consistent thermo-plastic constitutive model for unsaturated soils. The model also features a coupled THM approach of the water retention curve. Various couplings were studied separately and in combination in order to determine the significance of each. The same principle is applied to physical phenomena such as vapour diffusion. This study clearly highlights the effects that need to be taken into consideration for a correct assessment of EBS behaviour.

1. Introduction

The fate of high-level radioactive waste is of great importance to nuclear power plant operators and government agencies responsible for safety due to their extremely slow decay and the high risks associated with their management. Geological disposal is widely regarded as the safest option to alleviate any undue burden for future generations caused by this type of radioactive material (IAEA, 2006). This idea led to the development of the Engineered Barrier System (EBS) principle, which consists of using different layers of protection to insulate radioactive waste in all situations, from the short-term high-temperature situation to the very-long term scenario. Such a radioactive waste design makes use of a carefully chosen natural barrier (the so called *host rock*, even if host clays are also planned), as well as two additional layers of protection. One of these is the canister that contains the waste, which is fabricated from a metal, such as pure copper or a specific steel alloy. The second layer of protection is a buffer material that is designed to dissipate heat in a controlled manner in order to mitigate the risks from movements of the drift (host rock fracturation, seismic events) and to limit the possibility of radionuclide migration.

The aim of this paper is to identify the various couplings, identified from laboratory-scale experiments, that are the most relevant to a full-scale EBS. The analysis takes into account both the evolution of the physical processes and the physical quantities relevant for the design of the EBS. The paper focuses on the behaviour of the buffer material, as this is the location of the most complex and physically coupled thermo-hydro-mechanical phenomena. The buffer material most commonly used in EBS designs is bentonite, either compacted as blocks or in pellet form (NAGRA, 2002; Karnland et al., 2011). Although they behave differently, these two forms of bentonite share a large number of their main characteristics (Laloui et al., 2008); they both exhibit a very low permeability, a highly variable thermal conductivity, an initial unsaturated state, and swelling characteristics.

The various processes that occur in the buffer are first outlined, with an emphasis on the coupled phenomena, as well as the necessary constitutive equations that describe them. This section includes the diffusive aspects (thermal and hydraulic behaviour), as well as their coupling using a mechanical constitutive model. Next, the chosen mechanical constitutive model is described, which is the ACMEG-TS model (François and Laloui, 2008), an elasto-thermoplastic model that uses the framework of generalized effective stress for unsaturated soils. In the second section, a case study is described that is designed to represent a generic EBS design with limited site effect, in order to underline the constitutive variations. This case study is simulated using the described constitutive equations in a finite element code. The results obtained for a base case are presented. Finally, results from a sensitivity analysis, with coupled phenomena turned on or off and with coupling parameter variations, are shown.

The case study under consideration is that of a single canister enclosed in a hole that is excavated without access drift. This choice allows the elimination of the site effects due to the drift and gives a better analysis of the effects of the modelling modifications. The geometry and heat dissipation are based on the Swedish proposal for an EBS (Karnland et al., 2011), and the canister emits heat

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according to the decay of a real high-level waste canister. The geometry of the vertical deposition hole is shown in Fig. 1. As in the planned repositories, holes are excavated with a regular pattern, 400 m below the surface; therefore the modelled host rock radius is small (8.74 m) while a sufficient height is needed to avoid boundary effects (100 m).

2. Coupled processes in an EBS

2.1. Physical description

With the exception of the canister, the materials involved in the problem are porous media. The description of diffusive processes in such media has been treated with a variety of approaches such as the theory of mixtures (Bowen, 1982), which is used here. This approach separates species and phases into constituents for the mass balance equations, allowing a clear identification of the phase change quantity, which cancels out in the balance equations of the chemical species, using the compositional approach (Panday and Corapcioglu, 1989; Collin et al., 2002). The diffusive model presented in Section 2.2 is used for both the host rock and bentonite buffer.

In order to understand the various processes involved, it is necessary to define the extreme conditions that are encountered. The temperatures considered in this study are between 15 and 80 °C, which are the design criteria for some EBSs (Karnland et al., 2011). Higher temperatures up to 100 °C have been shown to increase the significance of vapour transport without introducing additional phenomena (Dupray et al., 2013). The host rock is considered to be saturated, and acts as a permanent supply of water to the initially unsaturated buffer. The first two processes are thus an increase in temperature adjacent to the canister (diffusion of decaying radionuclide heat) and water exchange at the boundary between the saturated host rock and unsaturated buffer materials. The heat generated is thought to be capable of provoking further drying of the unsaturated buffer, as well as vapourisation of water. In terms of modelling, this implies that the water retention model should be able to reproduce the effect of temperature on the retention capacity.

Changes in liquid water content strongly influence the thermal conductivity, as well as the heat capacity, of the porous media. Bentonite is extremely affected by this phenomenon (Börgesson et al., 2001). The degree of saturation will have a huge effect on the gas and liquid relative permeabilities of the porous medium. The diffusion of vapour created close to the canister should also be modelled, while the Richards' approximation is used to model vapour diffusion in a static gas phase; Wang et al. (2011) demonstrated the use of this solution to provide good results in full-scale simulations. Convective heat flow can also be induced by fluid flows and should be taken into account, for both vapour and liquid water.

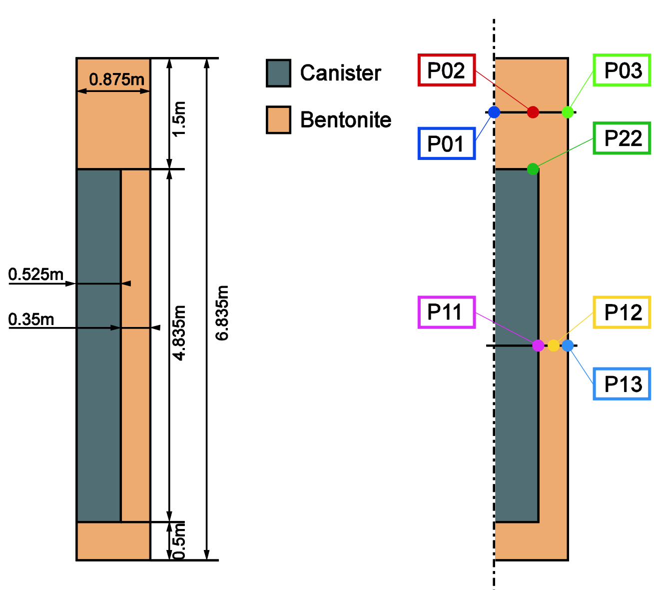

Fig. 1. Geometry of the considered deposition hole, location of monitoring points.

Another aspect that influences the diffusive behaviour of the buffer is the effect that mechanical changes (strains) have on both water flow and thermal behaviour. The thermal behaviour is affected by density changes during compaction or dilation, while volumetric strains affect the intrinsic permeability of the buffer material. On the other hand, water migration in the media can be affected by changes in permeability caused by mechanical strains. When talking of a clayey material such as bentonite, this interpretation is not the only one possible and the concept of film transport, which depends on temperature and water content may also be used (Yong et al., 2010). This aspect is neglected here due to the small range of validity of this concept (from 10 to 20% degree of saturation according to Winterkorn (1960)).

Thermo-hydro-mechanical couplings affect not only the diffusive part of the model, but also the mechanical one. The most well-known effects are the increase in strength that is induced by drying, and the changes in the swelling behaviour at high temperatures (Villar and Lloret, 2004). These experimentally-observed effects are taken into account directly in the constitutive model and are detailed in Section 2.3.

2.2. Coupled diffusive model

2.2.1. Water species

As stated previously, the compositional approach is used, as implemented by Collin et al. (2002) in the software *Lagamine*, that is also used for this study (Charlier et al., 2001). This approach allows writing the mass balance equation for water in a straightforward manner, including terms for storage of both liquid and gaseous water, advective flow of water, non-advective flow of vapour and source terms:

$$\underbrace{\frac{\partial}{\partial t}(\rho_w n S_r) + div(\rho_w \mathbf{f_l}) - Q_w}_{\text{Liquid water}} + \underbrace{\frac{\partial}{\partial t}(\rho_v n(1-S_r)) + div(\mathbf{i_v}) - Q_v}_{\text{Water vapour}} = 0 \tag{1}$$

where ρ_w and ρ_v are the bulk density of liquid water and water vapour; $\mathbf{f_l}$ is the macroscopic velocity of the liquid phase; $\mathbf{i_v}$ is the non-advective flux of water vapour, itself the opposite of dry air flux; S_r is the degree of liquid saturation, and n the porosity. The term $\rho_w n S_r$ is the storage term for liquid water. No gas flow appears, as per Richards' approximation.

Among these terms, the liquid water flow is defined by the generalized Darcy's law for porous media:

$$\mathbf{f_l} = -\frac{k_{r,w} k_{int}}{\mu_w} \mathbf{grad}(p_w) \tag{2}$$

where p_w is the liquid water pressure, $k_{r,w}$ the relative permeability to water, k_{int} the intrinsic permeability and μ_w the dynamic viscosity of liquid water. The relationship between the relative permeability and degree of saturation is defined according to the properties of each material. The intrinsic permeability depends on porosity through a Kozeny–Carman relationship:

$$k_{int} = k_{int,0} \left[\frac{n/n_0}{(1-n)/(1-n_0)} \right]^{\eta} \tag{3}$$

where $k_{int,0}$ is the intrinsic permeability at the initial porosity n_0 and η is a material parameter. This relationship and the storage term in Eq. (1) define one side of the hydro-mechanical coupling.