Coupled Hydro-Mechanical Model of Bentonite Hydration and Swelling

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Abstract. This paper deals with the modelling of coupled hydro-mechanical processes at the buffer and host rock interface (bentonite and granite) in the context of the safe disposal of spent nuclear fuel. Granite, as one of the barriers, includes fractures which are the source for hydration of bentonite and its subsequent swelling. It affects the mechanical behaviour and possibly the stability of the whole system. A non-linear solution for the stress-deformation problem with swelling was developed. This solution is coupled with the non-linear diffusion problem (for unsaturated flow). The swelling is defined using a coefficient dependent on water content according to literature data, with the effective Young's modulus decreasing close to zero corresponding to the plastic state. Results confirm the expected non-uniform saturation, swelling, and stresses in bentonite and small contribution to a fracture displacement.

1. Introduction

One of the challenges in the safety analysis of engineered barriers in spent nuclear fuel repositories is the representation of bentonite hydro-mechanical behaviour in numerical models. Typically, thermo-hydro-mechanical(-chemical) processes in bentonite e.g. the interaction of bentonite and the host rock (fractured granite), are equally important, requiring the joining of the two disciplines of soil and rock mechanics.

The aim of many studies in the literature is to interpret in-situ experiments, which simulate the repository conditions, including full-scale cases with bentonite-rock interaction. On the other hand, the inhomogeneity of water transfer between the host rock and the bentonite has not been a main issue. Many experiments concentrated on the behaviour of bentonite under controlled conditions of saturation (e.g. a water injection layer). In addition, generic predictions of the repository operation are typically simplified for homogeneous conditions.

Recent detailed modelling studies have been performed with the data from the Prototype Repository (e.g. Malmberg and Kristensson [1], Thomas et al. [2] and Chen and Ledesma [3]) and the Bentonite-Rock Interaction Experiment (BRIE) at the Äspö underground laboratory in Sweden. The BRIE experiment investigates the interaction between the rock with few fractures and bentonite in a borehole – the water exchange across the bentonite-rock interface. The presented model is a generic case based on the conceptual ideas of both. Compared to the BRIE (hydraulic-only), hydro-mechanical coupling is considered in this case. Compared to the Prototype, a schematic single-fracture intersection instead of a complex inflow matrix and isothermal conditions was used.

2. Model concept

The model concept is based on the hydro-mechanical (HM) coupling of non-linear diffusion (water transport) and non-linear elasticity. The diffusion equation with non-linear diffusivity, suggested by Börgesson [4], represents an equivalent expression to Richards' equation for the solution of flow problems in partly saturated conditions. The non-linear elasticity approximates a transition from the elastic to plastic properties of bentonite. The one-directional coupling is controlled by a swelling and a saturation-dependent Young's modulus. The diffusion equation with non-linear diffusivities (obtained from the retention curves) is different for bentonite (1) and different for the rock or the fracture (2).

$$\frac{\partial S_l}{\partial t} = \nabla \cdot \left[\left(\frac{k}{n \cdot \mu} \cdot S_l^{\,3} \cdot \frac{P_0}{\lambda} \cdot (1-\lambda) \cdot \left(S_l^{-\frac{1}{\lambda}} - 1 \right)^{-\lambda} \cdot S_l^{\frac{-1-\lambda}{\lambda}} \right) \nabla S_l \right] \tag{1}$$

$$\frac{\partial S_l}{\partial t} = \nabla \cdot \left[\left(\frac{k}{n \cdot \mu} \cdot \sqrt{S_l} \cdot \left(1 - \left(1 - S_l^{\frac{1}{\lambda}} \right)^{\lambda} \right)^2 \cdot \frac{P_0}{\lambda} \cdot (1-\lambda) \cdot \left(S_l^{-\frac{1}{\lambda}} - 1 \right)^{-\lambda} \cdot S_l^{\frac{-1-\lambda}{\lambda}} \right) \nabla S_l \right] \tag{2}$$

where S_l is the degree of saturation, k the permeability of the medium, μ the dynamic viscosity, n the porosity, P_l the water pressure, P_0 and λ are van Genuchten retention curve parameters and t is time. Although the rock and the fracture are saturated at the simulation beginning, the equation defines them as variably saturated.

The mechanical part is governed by (formally) standard equations of elasticity partly with a non-linear Young's modulus. For the rock and the fracture (particular meaning explained below), the Young's modulus is a constant. For the bentonite, the Young's modulus is dependent on saturation, according to Figure 1. The HM coupling – the relation between the hydration and swelling of bentonite is described by a coefficient of volume expansion depending on the degree of saturation according to Börgesson [5]. The dependence of the volume expansion coefficient on the degree of saturation also indicates a stepped increase in bentonite volume at 80% hydration (explained in 3.2). Thus, potential displacement along the fracture is caused by bentonite swelling. With the simplification of the excavation geometry on the borehole only (no tunnel), it is not possible to determine realistic stresses in the rock and the model is defined as the swelling-induced stress change evaluation only. Since we cannot distinguish the stress states with respect to a fracture strength condition, a possible range is covered by two generic limit cases – elastic and slip – distinguished by an effective modulus (section 3.3.).

3. Solved model

The idea of the model concept is based on previous simpler models in 2D axisymmetric geometry with a horizontal fracture described in Skarydova and Hokr [6]. The problem is extended to 3D geometry with a particular case of a more general fracture position (with real orientation according to the BRIE experiment), which causes inhomogeneous inflow to the borehole and non-uniform bentonite hydration. The model consists of a block of rock (granite) with a separate cylindrical borehole filled with bentonite.

3.1 Model geometry and material properties

The granite block dimensions are 10 × 10 × 13.5 m and the bentonite cylinder in the centre has the radius of the base 15 cm and the height 3.5 m, see Figure 2. The fracture in the rock is represented by a 3D entity with different material properties and a thickness of 10 cm. This larger size (not corresponding to the real aperture) is considered due to the finite-element mesh construction; it represents a real fracture by effective properties – the overall transmissivity corresponding to a realistic aperture in μm magnitude and the shear stiffness of planar discontinuity expressed in GPa/m. The position of the fracture is described by three parameters: strike = 139.5°, dip = 62.8° and the vertical coordinate at the borehole axis (z = 2.73 m).

The two different forms of non-linear diffusivity referred according to (1) and (2) represent the hydraulic parameters of the rock or fracture and bentonite. The dependence on the degree of saturation is specified by the parameters in Table 1. The diffusivity of the granite and the fracture is described by the same relation; the difference is in the higher value of permeability of the fracture material according to its real behaviour (retention curve parameters are identical for both materials). The diffusivity of the bentonite is expressed by a non-linear relation that shows the different capability of bentonite to soak water with varying water content.

The specific material properties necessary for mechanical model description of bentonite are referred to in Figure 1. Bentonite swelling – mechanical expansion is expressed by a coefficient of volume expansion dependent on the degree of saturation. The swelling is the main contribution to hydro-mechanical coupling, as an expansion proportional to water content (saturation). No expansion is considered for rock and the fracture. The elastic parameters of granite matrix are typical values from literature. There are two variants of material which represents fracture – one with larger value of Young's modulus for the elastic regime below a strength limit of the discontinuity (denoted as stiffness 1) and the second with smaller value for the slip regime, as linearization of elastic and plastic parts in a chosen range (stiffness 2).

3.2 Boundary conditions

Full saturation is prescribed on all outer boundaries of the computational domain (rock and fracture outer boundaries) as the hydraulic boundary condition, which represents an unlimited source of water. It is assumed that the granite and the fracture are fully hydrated at the beginning of the process (initial condition of S_l = 100 %) and the initial saturation in the borehole is 36 %. Zero displacement in the normal direction of the appropriate coordinate axis is also prescribed on all outer boundaries. It represents the concept limited to the evaluation of the stress and deformation change resulting from the swelling only.

The model is simulated in the multi-physical system ANSYS 13.0 [7], using a standard heat transfer equation as an analogy to diffusion equation. The temperature represents the degree of saturation and thermal conductivity is used for the diffusion coefficient. The mechanical part is solved with standard elasticity equations with a non-linear Young's modulus and swelling is represented by a thermal expansion coefficient. Although the problem could be classified as a small problem (50 thousand elements), the solution was time consuming (about 8 hours), thus a finer mesh with a large number of elements was not used.

Table 1. Material properties used in model with two variants of Young's modulus of the fracture (stiffness 1 and stiffness 2 – in brackets)

	Material parameter	Unit	Bentonite	Granite	Fracture
P_0	Retention curve parameter	[MPa]	9.23	1.74	1.74
λ	Retention curve parameter	[1]	0.3	0.6	0.6
k	Permeability	[m^2]	$9.5\cdot10^{-21}$	$9.0\cdot10^{-22}$	$2.5\cdot10^{-15}$
n	Porosity	[1]	0.438	0.003	0.003
μ	Dynamic viscosity	[Pa·s]	10^{-3}	10^{-3}	10^{-3}
E	Young's modulus	[Pa]	Figure 1	$6.1\cdot10^{10}$	$6.1\cdot10^{9}$ ($6.1\cdot10^{5}$)
v	Poisson's ratio	[1]	0.3	0.3	0.3

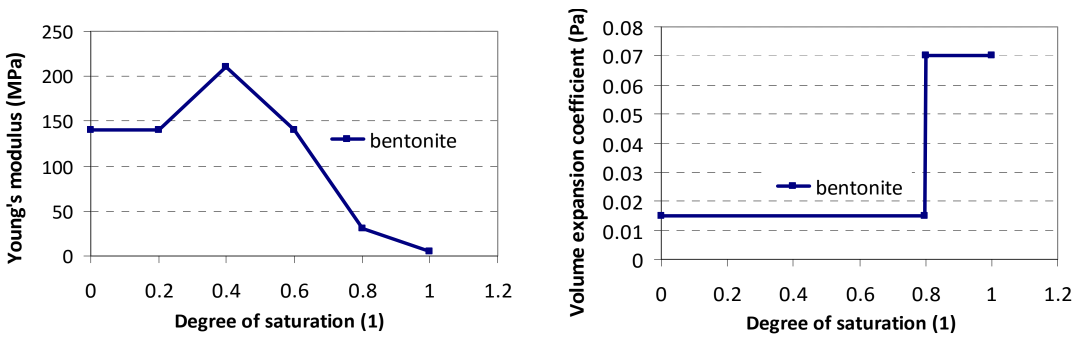

Figure 1. Dependence of Young's modulus and volume expansion coefficient S_l for bentonite

4. Results and discussion

It is possible to describe the problem solved in terms of hydration and with respect to the change of mechanical behaviour during the saturation process. Bentonite in the borehole is hydrated in two different ways: through the fracture and through the rock matrix. According to the results of the simulation, it is obvious that the hydration through the rock matrix has a significant influence on bentonite saturation in this case (see the detailed quantification in Skarydova and Hokr [6] and [8] for a similar model setup). Due to the fracture position, the bottom part of the borehole is hydrated more quickly than the upper borehole section. The borehole with bentonite is largely hydrated within 3 years. The referred times for reaching different average degrees of saturation are: 50% in 150 days, 75% in 1.3 years, 85% in 2.3 years and 90% in 3.2 years.

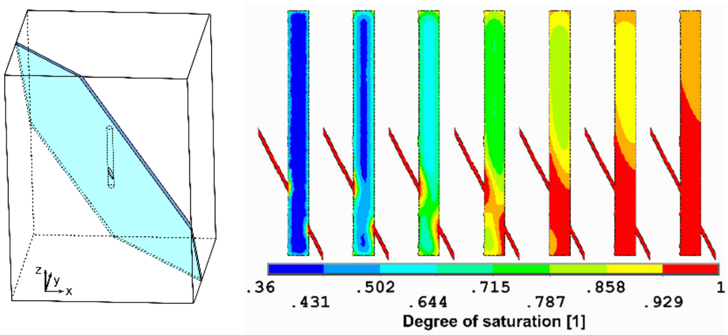

Figure 2. Geometry representation and the progress of S_l in bentonite in time (0.3 – 3.2 years)

4.1 Mechanical results for bentonite

The displacement vector components in the bentonite in x- and y- directions reach similar values while the z-component is lower, which corresponds to the saturation and swelling inhomogeneity in the radial direction. Maximum values of the displacement vector magnitudes are referred to in Table 2. Components of the stress tensor are compressive with the higher values at the top and bottom of the borehole. Distribution at the bottom is significantly unsymmetrical due to the fracture position. Components s_{xx}, s_{yy} and s_{zz} achieve similar maximum values, while the shear components are approximately five times lower with the dominant s_{xy} component.

4.2 Mechanical results for granite

The values of the displacement vector (Figure 3, Table 2) for granite are two orders of magnitude lower than for bentonite, which agrees with the difference of Young's modulus. Similarly to bentonite, u_z

values in granite are lower than u_x and u_y and on the contrary to bentonite, the maximum values of u_y are two times higher than u_x, corresponding to orientation of the fracture.

The distribution of the stress field in the rock is affected by the fracture – the maximum values of all the stress tensor components are located close to it. Compressive stress, in particular, reaches similar values for all Cartesian components. The most significant shear component is s_{xy} (as well as for bentonite). The two variants of the fracture effective stiffness differ in the resulting shear displacement by an order of magnitude. From the highest value at the borehole, it decreases quickly along the 0.5 – 1 m distance (2.54 μm for stiffness 1 and 6.58 μm for stiffness 2).

Table 2. Maximum (absolute) values of the total displacement, 1st principal stress and stress intensity factor for stiffness 1 and stiffness 2 (in brackets)

	u_{sum} [mm]	1^{st} principal stress [MPa]	stress intensity factor [MPa]
Bentonite	6.42 (13.40)	3.41 (4.13)	2.12 (2.13)
Granite	0.023 (0.15)	11.61 (39.37)	14.33 (42.39)

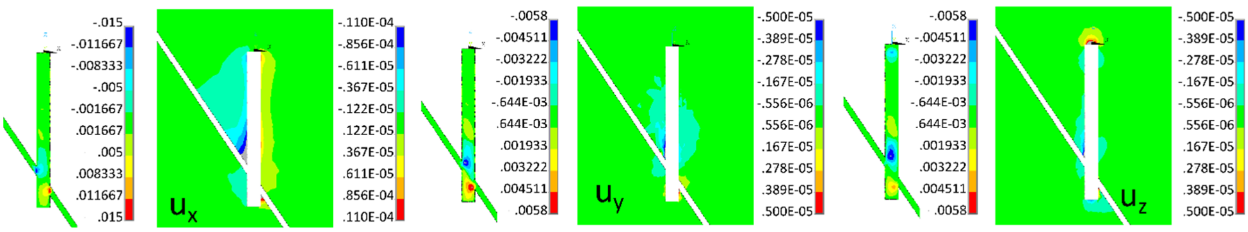

Figure 3. Displacement vector components (u_x, u_y, u_z (m)) in the sectional xz-view for fracture: ($E = 6.1 \cdot 10^5$ Pa). Different scale for rock and different for rock and fracture

5. Conclusions

Previously solved hydraulic model was coupled with swelling-induced stresses and displacements and extended to a fully 3D configuration. Although the repository concept works basically with swelling pressure as an isotropic value, possibly more complicated non-uniform bentonite load was demonstrated. But the consequences on its stability and integrity are not a subject of this paper. The mechanical effect on the rock is small but it is strongly concentrated in the fracture/borehole intersection with possible small-scale effects.

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