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ASPECTS OF THERMO-HYDRO-MECHANICAL SIMULATION OF A PROTOTYPE REPOSITORY IN FRACTURED ROCK

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ABSTRACT. A numerical investigation into the thermo-hydro-mechanical behaviour of a single deposition-hole in a nuclear waste repository is presented. In particular, two simulations are presented modelling first a deposition-hole in largely unfractured rock, and a second including a discrete fracture of 2m in radius intersecting the deposition-hole. The impact upon the hydraulic phase is discussed in detail and compared with experimental results from the Prototype Repository Project undertaken in Äspö, Sweden. It is found that the results correlate well, picking up the key differences in the saturation rates in the buffer material, especially in close proximity to the fracture represented.

1. Introduction

Nuclear waste resulting from civilian programs is a significant problem. Of this waste, low and intermediate level waste is being disposed of in below surface repositories. The high level waste, which is only 2% by volume, contains 92% of the radioactivity in the UK (CoRWM, 2006), hence produces a large amount of heat. Many countries, including UK, Sweden, Finland and France among others, have the intention of disposing of high-level nuclear waste utilising deep geological disposal. This concept involves containing vitrified waste or fuel rods in a copper canister containing a cast iron insert for strength. The canister is surrounded by a high-density expansive clay buffer and then placed into a deposition hole situated in bed-rock at approximately 400-500m depth.

For performance assessment of a geological repository it is important that the thermo-hydromechanical behaviour is known so that possible mechanisms for radioisotope escape can be identified and the structure can be appropriately designed. The hydraulic behaviour of the buffer material is complex, in part due to the expansive nature of the clay and the multi-level structure with the micro/macro-structure interaction affecting the overall behaviour. In addition, many suitable locations for geological disposal are made up of fractured crystalline rock which contains many discontinuities which are known to create highly anisotropic flow and preferential flowpaths.

In this paper the thermo-hydro-mechanical behaviour of a single deposition hole is investigated via numerical simulation to investigate the impact of relatively small fractures within a matrix of crystalline rock. Experimental behaviour of both deposition holes which intersect hydraulically active fractures and deposition holes which are locally contained within rock which does not have any hydraulically active fractures is found at the Prototype Repository Project (PRP). The PRP is a full scale mock-up experiment of deep geological disposal, designed to test on full-scale the thermo-hydro-mechanical performance of a repository system. It is located in the Hard Rock Laboratory in Äspö, Sweden and operated by SKB (Johannesson *et al.*, 2007).

Section 2 introduces the theoretical formulation, with section 3 proposing the modelling techniques and the specific simulations undertaken. In section 4 results are shown, compared briefly to experimental data and the concluding remarks are given in section 5.

2. Theoretical formulation

The materials contained within the model, rock, buffer and backfill materials, are assumed to be porous media. A coupled thermo-hydro-mechanical formulation is used, formulated in terms of the primary variables: pore-water-pressure, u_i , temperature, T, pore-air-pressure, u_a , and displacement, u. The flow variables are formed into governing equations using the principles of conservation of mass and the displacement is formed into a governing equation using equilibrium conditions. The soil deformation is governed using an elasto-plastic framework initially developed by Alonso *et al.* (1990).

The theoretical basis is formed into a standard Galerkin finite element form and developed into a bespoke computer code, COMPASS, whose details are described elsewhere (Thomas and He, 1997).

The resultant system of coupled equations expressed in matrix form is given as;

$$\begin{bmatrix} \mathbf{K}_{11} & \mathbf{K}_{TT} & \mathbf{K}_{1a} & -\\ \mathbf{K}_{T1} & \mathbf{K}_{TT} & \mathbf{K}_{Ta} & -\\ \mathbf{K}_{a1} & - & \mathbf{K}_{1a} & -\\ - & - & - & - \end{bmatrix} \begin{bmatrix} \mathbf{u}_{1s} \\ \mathbf{T}_{s} \\ \mathbf{u}_{as} \\ \mathbf{u}_{s} \end{bmatrix} + \begin{bmatrix} \mathbf{C}_{11} & \mathbf{C}_{TT} & \mathbf{C}_{1a} & \mathbf{C}_{1u} \\ \mathbf{C}_{T1} & \mathbf{C}_{TT} & \mathbf{C}_{Ta} & \mathbf{C}_{Tu} \\ \mathbf{C}_{a1} & \mathbf{C}_{aT} & \mathbf{C}_{aa} & \mathbf{C}_{au} \\ \mathbf{C}_{u1} & \mathbf{C}_{uT} & \mathbf{C}_{ua} & \mathbf{C}_{uu} \end{bmatrix} \begin{bmatrix} \dot{\mathbf{u}}_{1s} \\ \dot{\mathbf{T}}_{s} \\ \dot{\mathbf{u}}_{as} \\ \dot{\mathbf{u}}_{s} \end{bmatrix} + \begin{bmatrix} \mathbf{f}_{1} \\ \mathbf{f}_{T} \\ \mathbf{f}_{a} \\ \mathbf{f}_{u} \end{bmatrix} = 0$$
(4)

where \mathbf{K} , \mathbf{C} and \mathbf{f} are coefficients of the equations.

Temporal discretisation via a finite difference, implicit, mid-interval forward difference time stepping algorithm is used. The solution for the timestep n+1 can be expressed as;

$$\boldsymbol{\phi}^{n+1} = \left[\frac{\mathbf{B}^{n+\frac{1}{2}}\boldsymbol{\phi}^{n}}{\Delta t} - \mathbf{C}^{n+\frac{1}{2}}\right] \left[\mathbf{A}^{n+\frac{1}{2}} + \frac{\mathbf{B}^{n+\frac{1}{2}}}{\Delta t}\right]^{-1}$$
(5)

where A, B and C are the matrices of coefficients and are estimated using an iterative predictor - corrector algorithm and ϕ is the vector of variables.

3. Proposed model

To investigate the differential inflow into deposition holes into repository structures such as the PRP, an idealised axisymmetric domain has been modelled. A single deposition hole is virtually symmetrical therefore an axisymmetric analysis has been undertaken to reduce computational time. The domain is based upon the PRP, in particular, deposition-hole 1 (DH-1) which intersects a 2m radius fracture and DH-3 which does not. The results from experimental data both pre-emplacement of buffer material and post-emplacement show that there is a large differential inflow between these holes. Figure 1 outlines the idealised domain including the rock mass, buffer material and canister. The fracture contained in figure 1 is included in the simulation where a fracture intersects the deposition-hole and is excluded to simulate an intact rock.

A modified continuum finite element model is used to allow the bulk rock mass and particular discontinuities to be represented. In the main an effective continuum is used to include the intact rock and statistical distribution of small fractures. Larger fractures have been included explicitly which allows preferential and highly localised flow. The material parameters are modified for the fracture to allow a higher hydraulic conductivity.

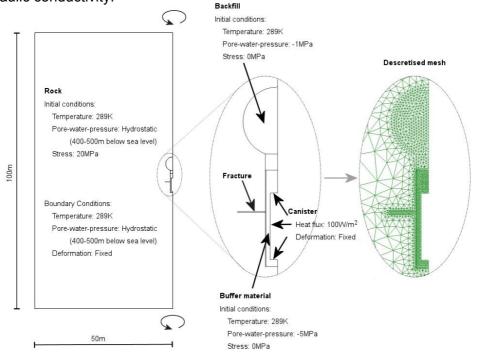


Figure 1. The model domain. Simulations performed both with and without the inclusion of the local fracture.

Figure 1 also shows the discretisation of the domain local to the canister and buffer material, identifying the initial and boundary conditions. It can be seen that the mesh is more detailed in and around the repository structure due to higher parameter gradients and a finer result resolution required. The analyses simulate 10 years performance and material parameters have been established from experimental results where possible.

The initial pore-water-pressure of the rock is assumed to be hydrostatic with the water table which is situated 400m above the top of the domain. While it is acknowledged that this will not be exactly the case due to the construction process and subsequent inflow into the repository structure, the rock is likely to still be largely saturated as the air in the repository is not able to maintain high negative pore-water-pressures. The suction of the buffer material is measured from the soil-water-retention-curve, a fitted van Genutchen relationship, and the reported initial water contents from manufacture (Börgesson *et al.*, 2002). The initial temperatures were as measured and the heat flux is maintained constant based upon the initial heat flux in the PRP. The heat from the canisters is simulated as a heat flux of 100 W/m^2 .

4. Results

Two simulations were performed, one without a fracture and one with a fracture. All other parameters were identical between the two analyses; hence they are able to demonstrate two things. The first, as to whether the key experimental features of such differences are able to be simulated and the second, to investigate the impact that discrete fractures may have in more detail than possible experimentally.

Results in the thermal field are almost identical and for the sake of brevity have not been reported on in detail. The temperature rises to 345K at the end of the analysis where an almost steady-state is reached. In reality this temperature field may be intersected by the temperature field from other deposition holes in close proximity.

The differences in the mechanical field are closely linked to the hydraulic results, as the material used in the buffer is highly expansive. Therefore, the hydraulic results are closely examined. Stresses were approximately 5MPa for the fractured rock and less than 1MPa for the unfractured rock.

Figure 2 shows a series of contour plots of the pore-water-pressure over time. Series (a) is unfractured and series (b) is fractured. It is clearly seen that the mid-section of the buffer material saturates quickly whereas the top and bottom sections saturate faster, but not as dramatically.

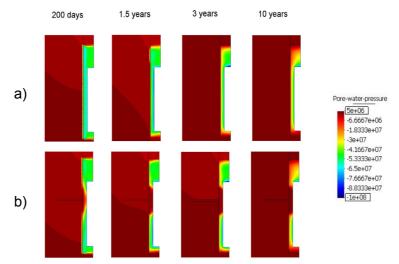


Figure 2. Contour plot of the pore-water-pressure, in Pa, for (a) the untractured rock and (b) the fractured rock.

These results can also be seen overlaid onto experimental results (Goudarzi and Johannesson, 2007) in figure 3. The results are from locations at the top of the bentonite buffer, the midsection, near to the location of the fracture and at the bottom. It must be noted that many of the sensors have stopped working and show some level of interference and uncertainty.

It can be seen that qualitatively the results are well simulated. The major difference, that the buffer saturates quickly at the mid-height, is well defined in the simulation. In the generally unfractured deposition-hole shown in figure 2a and 3a it is seen that some saturation occurs but at a relatively slow gradient. In the deposition-hole which contains the fracture slightly faster saturation occurs in the whole deposition-hole, but with a significantly lower gradient at the top and at the bottom of the buffer material. Slight quantitative discrepancies are likely to be due, in part, to a more complex network of fractures than represented existing for both simulations. The sensor at the bottom of the fractured sample seems

100				100				
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to saturate quickly and then begin to de-saturate before stopping working. It is possible that this sensor is not performing correctly or that local saturation is occurring.

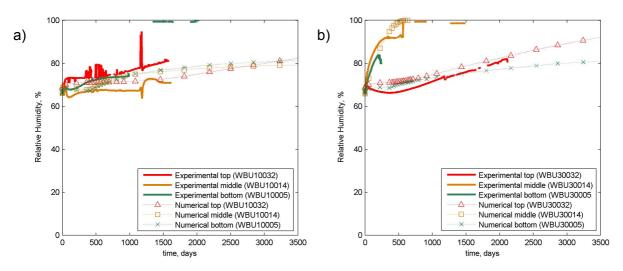


Figure 3. Exerimental and numerical results for inflow into (a) an unfractured deposition hole and (b) a fractured deposition hole.

5. Conclusions

A numerical model has been proposed to simulate the thermo-hydro-mechanical behaviour of a single deposition hole in a high-level nuclear waste repository in fractured rock. The key behaviour of the hydraulic field whereby the buffer saturates quickly where fractures intersect the deposition holes has been simulated and is found to reasonably match experimental results. It is this hydraulic behaviour that is a major driver for the mechanical behaviour.

6. Acknowledgements

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