- 1 Three-dimensional behaviour of a prototype radioactive
- 2 waste repository in fractured granitic rock.
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26 Abstract:

27 An investigation of the three dimensional coupled Thermo/Hydro/Mechanical behaviour of a prototype repository in fractured granitic rock is presented. The pre-placement behaviour of 28 29 the repository is first considered, making use of a full three-dimensional simulation of the 30 problem. An effective continuum approach, augmented with discrete features with a high hydraulic conductivity, is employed. The method adopted is found to be able to simulate 31 32 accurately the highly anisotropic flow regime observed at the pre-placement phase. The 33 major features of the full repository experiment under applied heating conditions were then successfully simulated. The range of buffer hydration rates, the thermal response of the 34 35 repository and the associated mechanical response were successfully simulated. Approaches to capture both the transient microstructural behaviour of the compacted bentonite (MX-80 36 37 type) and a MX-80 pellet material are incorporated. The repository behaviour was shown to 38 be strongly influenced by complex coupled processes, including interactions between the 39 system components. The adoption of a three dimensional modelling approach proved to be 40 essential in order to realistically simulate the behaviour of a repository incorporating 41 anisotropic flow behaviour. Finally potential impacts of the processes considered on 42 performance of the barrier system and in safety assessment are considered.

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53	Notation:	
54	b	parameter in soil water retention equation in table 2
55	C_{ps}	heat capacity of solid
56	G	shear modulus
57	k	cohesion parameter
58	k _{init}	initial hydraulic conductivity of the pellets
59	k _{inf}	final hydraulic conductivity of the pellets
60	K_l	unsaturated hydraulic conductivity
61	K _{feat}	hydraulic conductivity of the features
62	K_{pel}	hydraulic conductivity of the pellets
63	K _{sat}	saturated hydraulic conductivity
64	K _{swell}	hydraulic conductivity after water absorption
65	М	slope of the critical state line
66	n	porosity
67	p_0^*	effective preconsolidation stress of a saturated soil
68	p_c	reference stress
69	P_0	parameter in soil water retention equation in table 2
70	r	parameter controlling the maximum stiffness of the soil
71	S	suction
72	S_l	degree-of-saturation
73	S_{labs}	absorbed degree-of-saturation
74	S _{lA}	the degree-of-saturation at which homogenisation of the pellets begins
75	t	time
76	Tr	transmissivity
77	Т	temperature
78	u	displacement
79	u_a	pore-air pressure

80	u_l	pore-water pressure						
81	х, у, z	orthogonal directions						
82	α	parameter in soil water retention equation in table 2						
83	α_l	parameter representing the rate of movement of water between the macro and						
84	micro structure							
85	α_T	coefficient of thermal expansion						
86	β	parameter controlling the increase of soil stiffness with suction						
87	β_l	parameter in soil water retention equation in table 2						
88	β_p	parameter representing the rate at which pellet homogenisation occurs						
89	δ	parameter in unsaturated hydraulic conductivity equation in table 2						
90	$ heta_{res}$	residual water content						
91	θ_{sat}	saturated water content						
92	κ	elastic stiffness due to stress change						
93	κ_s	elastic stiffness due to suction change						
94	λ_T	thermal conductivity						
95	λ(0)	plastic stiffness due to stress change						
96	$ ho_s$	solid density						
97	σ	stress in the direction of the subscript						
98	τ	shear stress, plane defined by subscripts						
99	υ	Poisson's ratio						
100	ω_{abs}	parameter defining the proportion of absorbed pore-water						
101	\mathcal{O}_{abs}^{max}	parameter defining the maximum proportion of absorbed pore-water						
102	ω_{pel}	parameter representing the influence of homogenisation on the hydraulic						
103	conductivity							
104	Keywords: Numerical modelling, Partial saturation, Radioactive waste disposal, THM, 3D,							
105	fractured rock.							

106 **1 Introduction**

107 In recent years considerable progress has been reported in relation to an improved 108 understanding of the coupled thermo/hydro/mechanical behaviour of unsaturated soils (e.g. 109 Villar et al., 2005; Thomas et al., 2009). Such work has often been carried out as part of 110 major international programmes of research directed towards the safe disposal of High Level Nuclear Waste (HLW). Indeed a number of papers have appeared in the recent literature 111 112 comparing results from full scale experiments, carried out in underground research 113 laboratories, with those from numerical simulations based on recent theoretical advances. This paper continues that pattern, now in the context of the "Prototype Repository" 114 experiment carried out by Svensk Kärnbränslehantering AB (SKB), the Swedish Nuclear 115 116 Fuel and Waste Management Company, at the Äspö Hard Rock Laboratory.

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The Prototype Repository Project was instigated to investigate aspects of the repository system in an integrated manner (Svemar and Pusch, 2000). The project aims to replicate SKB's (Kärnbränslesäkerhet or Nuclear Fuel Safety) KBS-3 deep geological repository design in as realistic a set of conditions as possible, in respect to design, installation, geometry, materials, construction and environment. The exception is that the effects of HLW are simulated by use of heaters.

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125 The hydraulic performance of a repository, prior to emplacement of the heaters, buffer 126 material and backfill, is of importance as this represents both the boundary conditions of the 127 buffer material and the 'initial conditions' of the post-placement system. The overall performance of a repository structure has been shown to be affected by its hydraulic 128 129 performance (Thomas et al., 2003, 2009; Vardon et al., 2011). This hydraulic behaviour has 130 been well characterised via inflow measurement and hydraulic tests using drilled boreholes (e.g. Rhén and Forsmark, 2001). This detailed dataset offers a valuable opportunity to 131 132 investigate the behaviour of the system via numerical modelling.

The Thermo/Hydro/Mechanical (THM) behaviour of the repository is of importance for the containment and isolation of the waste as well as the onset of other processes, such as gas generation. The real behaviour is anisotropic and three-dimensional in nature and therefore has been represented as such throughout this work. The hydraulic behaviour of the rock provides the inflow of groundwater into the repository and therefore, in part, controls the resaturation behaviour, a key aspect of the THM behaviour.

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The Prototype Repository Project (PRP) is initially outlined in this paper, including the preplacement conditions and the experimental investigation of the rock. A three-dimensional numerical simulation of the pre-placement conditions is then presented, which includes the discrete fractures observed in the rock, allowing three-dimensional flow behaviour to be simulated. The THM behaviour of the prototype repository was then investigated.

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147 Previous attempts of work in this area have been presented by Cleall et al. (2006) and Chen 148 and Ledesma (2009). The former approach was able to realistically simulate pre-placement infiltration into some deposition-holes but could not capture, in full, flows to all the holes. 149 150 Post-placement conditions were analysed with two dimensional THM and three dimensional 151 thermo/hydraulic simulations. Overall the temperature domain was well represented. Some 152 realistic hydraulic results were obtained and limited consideration of the mechanical field was 153 made. The key conclusions were that three dimensional modelling was essential, the 154 representation of the fractured nature of the rock was required and the pelletised material was 155 not well understood. Chen and Ledesma (2009) utilised an approach using different 156 hydraulic conductivities in the rock around each deposition-hole to allow for differing in-flow 157 rates. Simulated thermal results correlated well, but very limited hydraulic results were 158 presented. Whilst both sets of authors were able to simulate selected parts of the experiment 159 successfully they presented limited comparison of results and recognised the value of three-

160 dimensional simulations. In neither case were fully coupled three dimensional THM analyses161 undertaken.

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In this paper, the previous approaches are extended to encompass large-scale three 163 164 dimensional simulations, undertaken to represent the overall behaviour of the prototype 165 repository. For reasons of conciseness and space limitations, only selected results are 166 presented here, with the data presented designed to give an overview of the results achieved. The THM model utilised in this work, COMPASS, has previously been presented in detail 167 168 (e.g. Thomas and He, 1997, 1998) and includes representation of coupled thermal, hydraulic, 169 air and mechanical processes. The governing equations are cast in terms of a primary 170 variable for each of the equations: pore-water pressure, u_l , temperature, T, pore-air pressure, 171 u_a , and displacement, **u**. The principle of conservation of mass is used for the governing 172 equations of moisture and air flow, conservation of energy for the flow of heat and equilibrium for the mechanical constitutive relations. Both liquid and vapour flow are 173 174 considered in the hydraulic governing equation, with vapour flow assumed to occur via diffusion due to temperature driven vapour concentrations in the buffer. Numerical solution 175 176 of the governing equations is achieved via the finite-element method for spatial discretisation 177 and the finite-difference method for temporal discretisation. A parallel Bi-Conjugate 178 Gradient solver is used to solve the system of equations (Vardon et al., 2011), with a 179 predictor-corrector algorithm used to allow for material non-linearity.

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181 2 Prototype Repository Project

The Prototype Repository Project (PRP) is a full-scale experiment designed to investigate the thermo-hydro-mechanical behaviour of a HLW repository. The experiment is designed to be more realistic than previous experiments (e.g. the Temperature Buffer Test (Hökmark et al., 2005) and the Canister Retrieval Test (Thorsager et al., 2002) at Äspö Hard Rock Laboratory (HRL); and the Buffer/Container Experiment (Thomas et al., 2009) and the Isothermal Test 187 (Thomas et al., 2003) at Atomic Energy of Canada's underground laboratory) and integrate 188 all aspects of the multi-barrier repository system including realistic setting within a real rock 189 mass at realistic depth. Consequently the experiment exhibits three-dimensional behaviour. In addition, the timescale that the project is designed for, up to 20 years, is unique and may 190 191 vield important information regarding time-dependent behaviour. Importantly the experiment 192 is situated in fractured rock that exhibits anisotropic flow phenomena. This rock mass has 193 been characterised via boreholes and hydraulic tests. The PRP is well described by both 194 Svemar and Pusch (2000) and Johannesson et al. (2007). It is located at the edge of the HRL 195 facility at 450m below sea level. A schematic of the repository itself is shown in figure 1. It 196 is made up of two sections, one with four deposition-holes and the second with two, spaced 197 6m apart and drilled vertically and numbered from 1 to 6 as shown. The deposition-holes, as 198 indicated in figure 2, are filled sequentially with high density Wyoming bentonite blocks 199 (MX-80) surrounding the canister containing heaters at placement. Between the bentonite blocks and the canister is initially a 10mm gap and between the bentonite and the rock is a 200 201 gap (~50mm) which is filled with high density bentonite pellets. The tunnel and remaining 202 1000mm of the deposition-holes contain backfill, which is a crushed rock and bentonite mix 203 (70/30% by weight). A concrete plug was constructed between the two sections and another 204 isolating the project from the rest of the tunnel complex. The plugs were designed to 205 withstand the stresses and pressures that the system was likely to create.

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The pre-placement stage of the project starts with the construction of the tunnel and finishes when emplacement of buffer material, backfill and canisters begins. Measurements have been taken during this time period enable the rock to be characterised, numerical models to be calibrated and give an indication of initial conditions. Rhén and Forsmark (2001) present the collated data. The rock surrounding the PRP has been characterised at a relatively high resolution. Thirty-nine boreholes were drilled, and in 33 of these detailed hydraulic measurements were made. This has allowed the observation of both the characteristics of the

214 rock mass and the identification of specific features, such as local highly hydraulically 215 conductive fractures. In addition to the use of boreholes, the surface of the tunnel and 216 deposition-holes has been mapped and the hydraulically active areas identified. The inflow 217 rates into the tunnel and deposition-holes have also been monitored, with the results shown in 218 figure 3(a) and 3(b) respectively. The most important feature of these measurements is that 219 the inflow into Deposition-Hole 1 (DH-1) is much greater than into any of the others. Stress 220 measurements were also taken in one borehole to gain knowledge of the existing stresses with 221 the values reported in section 5.2.1.

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223 The fractures in the tunnel have been mapped using various techniques e.g. standard 224 mapping, laser scanning, Borehole Image Processing System (BIPS) Television (TV)-logging 225 (unsuccessfully) and Ground Penetrating Radar (GPR) (Patel et al., 1997). Importantly, the 226 hydraulically active features have been identified (Patel et al., 1997). The deposition-holes were mapped in the same manner; DH-3 was not identified to have any hydraulically bearing 227 228 fractures, unlike for example DH-1 and DH-5. A similar number of hydraulically bearing fractures were identified in DH-1 and DH-5, with DH-1 having a significantly larger inflow 229 230 rate. A tentative conclusion can be drawn, that the majority of the flow occurs through these 231 hydraulic features and that the flow generally diffusing through the rock matrix is small in 232 comparison, although the rates through the fractures may highly variable. A fracture 233 mapping of the tunnel (after Rhén and Forsmark, 2001) is shown in figure 4 where all 234 fractures have been mapped and hydraulically active fractures identified. Two areas of large inflows, denoted Area 1 and Area 2, have been identified and shaded. A more complete 235 236 overview of the drilling and testing regime can be found in Rhén and Forsmark (2001).

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Following the mapping, drilling and hydraulic tests the transmissivity of the rock and hydraulic connectivity was estimated and a number of key hydraulic features hypothesised by Rhén and Forsmark, (2001). These are detailed in Table 1 and diagrammatically included in 241 the domain visualisation in figure 5. It has been initially hypothesised by Rhén and Forsmark 242 (2001) that these features have circular shapes, with the coordinates quoting the centre of the 243 feature. Alternative shapes have not been utilised and may affect the results, due to the change in surface area and connectivity with other model features. However, analysis of this 244 245 aspect is beyond the scope of the work. The fact that some deterministic features have been 246 identified does not, by default, suggest that the remainder of the rock mass is not fractured, 247 but only that during the tests, significant identifiable preferential flow directions have not 248 been recognised in those regions. The sampling process uses a discrete number of boreholes 249 to identify these features and as such, some features are likely to be missed, but those of 250 reasonable size and proximity to the tunnels are likely to have been identified.

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252 Area 2, highlighted on the tunnel fracture map, figure 4, shows a region with a well defined 253 fracture which is hydraulically active and coincides with the intersection between the tunnel 254 and the proposed South major fracture. However, Area 1, highlighting a large water flow 255 into the tunnel and another well defined fracture, via surface fracture mapping, does not coincide with any deterministic feature proposed by Rhén and Forsmark (2001), although is 256 257 close to the South major fracture and it is possible that it may have some interaction. An 258 additional feature of hydraulic conductivity is proposed to allow the impact of increased 259 permeability in this region to be assessed, for convenience named Region 1.

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In the post-emplacement phase each of the deposition-holes, contains a copper canister inclusive of iron over-pack and heaters, compacted MX-80 bentonite buffer and pelletised MX-80 buffer material. The configuration is shown in detail in figure 2. The tunnel is backfilled with a mixture of crushed rock and bentonite and sealed between sections 1 and 2 and at the end by means of a concrete plug. A large quantity of data has been collected during the post-emplacement phase of the experiment (e.g. Goudarzi and Johannesson, 2007). Figures 6 and 7, for example, show data collected from DH-1 and DH-3. The highly

268 anisotropic and locally varied flow, apparent in the deposition tunnel and holes during the 269 pre-placement stage, results in the buffer in DH-1 resaturating at a faster rate than other 270 deposition-holes (Johannesson et al., 2007). All deposition-holes exhibit water content variations from a hot dry side to a cooler wet side of the buffer, before full saturation. The 271 272 thermal response is driven by the heat flux from the canisters with peak temperatures located 273 in DH-1 in the centre of section 1. In general, peak temperatures for drier deposition-holes 274 are higher than for wetter deposition-holes, as expected. Swelling pressures increase with 275 hydration, rising to up to $\sim 7MPa$ in locations where full saturation has occurred. However 276 observed patterns in pressure development are complex and their reliability has been 277 questioned due to possible arching effects, local contact and stress cell installation (e.g. Chen 278 and Ledesma, 2009). Finally, in the backfill a trend of saturation has been measured, with the 279 fastest rates found close to DH-1.

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3 Simulation approach

282 **3.1 Domain**

283 The information from the site data and the modelling strategy have been used to create a 284 geometric model of the domain for the pre-emplacement condition i.e. an empty tunnel and 285 deposition-holes within a rock mass, shown in figure 1, with the whole domain shown in figure 5(a) and details of the fractures and Region 1 shown in figure 5(b) - 5(d). The domain 286 287 has been chosen to extend approximately 50m away from the repository in all directions, to 288 ensure the effective deployment of the boundary conditions. To check that this is achieved 289 the hydraulic flux has been monitored at the domain edge. In addition, a single analysis has 290 been undertaken with a domain 100m away from the repository in all directions with only 291 negligible differences in any results (less than 1%); this has not been presented in this paper. 292 The total domain size is therefore $100 \times 100 \times 160m$ with the 160m dimension being along 293 the length of the tunnel. Linear tetrahedral elements have been used, allowing for irregular 294 shapes and enabling areas of complex geometry and great spatial variation of results to be

295 modelled with a fine mesh resolution, while areas which are expected to have little variation 296 of results and less complex geometry can have a significantly coarser mesh resolution. When 297 discretised the model has 484,954 tetrahedral elements and 86,414 nodes for the pre-298 placement conditions and 920,983 elements with 163,240 nodes for the post-placement, this 299 mesh has been checked for spatial convergence.

300 3.2 Material parameters

301 Material parameters and material behaviour relationships are summarised in table 2. As 302 noted by Chen and Ledesma (2009), gas pressures are likely to be small as temperatures are 303 not anticipated to be higher than 80 $^{\circ}C$ so advective gas transport is neglected. Where gas or 304 pore-air pressures are required in the formulation a constant of atmospheric pressure is used.

305 3.2.1 The host rock

306 The host rock is a complex fractured material made up from, in the main, Äspö Diorite. The 307 material is highly fractured with fractures and joints generally filled with chlorites, calcite and epidote and considered tight (Patel et al., 1997). The average density is 2770 kg/m^3 with 308 309 the porosity reported as being 0.005±0.002 (Dahlström, 1998; Patel et al., 1997). Discussion 310 of hydraulic material parameters for the crystalline rock in the Äspö area where the PRP is 311 situated is well documented (for example summarised by Rhén and Forsmark, 2001). The 312 parameters required for the analysis are the hydraulic conductivities of the 'intact rock', that 313 is the rock matrix including the background distribution of fractures, and the hydraulic 314 conductivity of the identified hydraulically conductive features and the associated porosities. 315 The rock is considered to be saturated throughout the pre-emplacement stage therefore no variation with degree-of-saturation is required. The values of hydraulic conductivity for the 316 317 'intact rock' were found, via experimentation, to have a wide range and were spatially variable. The range of values was found to be from 10^{-5} to 10^{-13} m/s. It has been conjectured 318 319 that the conductivity will be anisotropic due to geological processes (Rhén and Forsmark, 320 2001), however statistical confidence limits do not observe significant differences at the 90 321 percentile confidence limit (Vardon 2009). Other works show similar findings and wide

range of possible hydraulic conductivities, e.g. Rhén et al. (1997). A conductivity, at the lower end of the mid-range of experimentally determined conductivities, of 5×10^{-12} *m/s* will be used and the more significant deterministic hydraulic features included explicitly.

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326 The hydraulic features have been represented as areas of higher hydraulic conductivity than 327 the bulk rock mass. These higher hydraulic conductivities have been calculated from 328 transmissivities (Rhén and Forsmark, 2001), using a standard fracture thickness for modelling purposes of 0.1m for the major fractures and 0.05m for the minor fractures. The derived 329 330 values of hydraulic conductivity for the fractures are summarised in table 1. It should be 331 noted that the fracture thicknesses, whilst reasonable, are arbitrary and serve only to allow 332 representation of the fracture. There is little evidence to indicate the size or transmissivity of 333 the identified region of high hydraulic inflow into the tunnel, *Region 1*, therefore, a region 334 has been included within the geometric model, with the hydraulic conductivity of the major fractures. Unsaturated hydraulic conductivity and water retention behaviour, incuding 335 336 parameterisation, is based upon the approach of Gens et al. (1998) for granite. A heat capacity of 750 J/kgK is adopted, based upon Patel et al. (1997), and Dahlström (1998) 337 338 quotes the thermal conductivity as a constant 2.5 W/mK. A linear elastic mechanical model is 339 utilised for the host rock due to the relatively low stresses applied from the buffer material. 340 For Poisson's ratio, v, and shear modulus, G, values of 0.25 and 27,600 MPa are adopted 341 (Delin et al., 1995; Stille and Olsson, 1996).

342 **3.2.2 MX-80 bentonite**

The buffer material is highly-compacted sodium bentonite clay, known as MX-80. Blocks of buffer material were installed in rings, cylinders and bricks depending on location. They are designed to give a homogenised pattern of final dry density after rehydration and swelling. The installed average porosities were 0.4, 0.36 and 0.38 for the cylinders, rings and bricks, respectively (Börgesson et al., 2002). The heat capacity and thermal conductivity of MX-80 were determined by Börgesson and Hernelind (1999), with the heat capacity reported as 800 349 J/kgK. The thermal conductivity, λ_T , (W/m/K) was found to vary with degree-of-saturation, 350 S_b as:

$$\lambda_{T} = 0.3 \qquad S_{l} \le 0.2$$

$$\lambda_{T} = 1.5S_{l} \qquad 0.2 < S_{l} \le 0.8 \qquad (1)$$

$$\lambda_{T} = 0.8 + 0.5S_{l} \qquad 0.8 < S_{l} \le 1.0$$

352 An elasto-plastic model (Alonso et al., 1990) has been adopted to represent the mechanical 353 behaviour of the bentonite. The elastic and plastic stiffness due to stress change, κ and $\lambda(0)$, 354 were found based upon experimental evidence collated by Pusch (2001) after Börgesson et al. 355 (1993) as 0.0245 and 0.238. The parameters for the relationship defining plastic stiffness for any suction ($s = u_a - u_w$), r and β , were found experimentally by Lloret et al., (2003) to be 0.9 356 and 1.0 respectively. Following Alonso et al. (1990) the reference stress, p_c , was defined as 357 atmospheric pressure. The effective preconsolidation stress of a saturated soil, p_0^* , is 358 estimated based on the maximum preconsolidation pressure applied to the sample during 359 360 construction of the blocks (100MPa) and the initial suction yielding a value of approximately 361 The mechanical behaviour of bentonite due to suction is based upon work 45*MPa*. undertaken by Lloret et al. (2003). The elastic stiffness due to suction change, κ_{s} , was found 362 363 to be 0.075 with little or no plastic behaviour exhibited in the suction range considered (up to 364 500MPa). Therefore the suction yield surface was not considered. A shear modulus, G, of 365 10MPa is adopted following Cleall et al. (2006). Following experiments undertaken by 366 Börgesson et al. (1995) the slope of the critical state line, M, can be shown to be 0.358, with a first estimate of the cohesion parameter, $k=5.6\times10^{-3}$, based on the approximate cohesion of 367 56kPa with the samples at approximately $1 \times 10^7 Pa$ suction. Limited thermal expansion will 368 369 take place, based largely on the amount of water in the sample (Börgesson et al., 1995). As 370 this is likely to be significantly less that the expansion due to suction a constant based on average water content is used of, thermal expansion, $\alpha_T = 1 \times 10^{-4} K^{-1}$. A saturated hydraulic 371 372 conductivity, determined from experimental results by Börgesson and Hernelind (1999) and 373 Villar et al. (2005) has been employed. The moisture-retention behaviour is represented using

a van Genutchen relationship fitted to experimental data presented by Börgesson andHernelind, (1999).

376 3.2.3 MX-80 pellets

Very limited experimental data exists for MX-80 pellets. Hoffmann et al. (2007) presented a 377 378 series of experiments exploring the hydro-mechanical behaviour of such pelletised materials 379 and these have been further investigated more recently by Alonso et al. (2011). For 380 mechanical model parameters Hoffman et al. (2007) presented some initial results and recommends an increase in stiffness with application of stress. A sensitivity analysis for $\lambda(0)$ 381 382 has been undertaken using experimental results from the Canister Retrieval Test (CRT) 383 (Thorsager et al., 2002) yielding a value of 0.6 for the homogenised pellet region. In the 384 absence of other data, thermal behaviour will be assumed to be similar to that of the MX-80 385 bentonite buffer material.

386 3.2.4 Backfill

The backfill material is a mixture of crushed rock from the tunnel excavation (70%) and 387 388 bentonite (30%) and is installed in compacted layers (Johannesson et al., 2007). The 389 bentonite is a converted sodium bentonite originating from Milos, Greece. The water content at installation was 12% and a porosity of 0.363 was determined consistent with the dry-390 391 density of $1.65g/cm^3$ (Börgesson et al., 2002). The saturated hydraulic conductivity was found to be 1.5×10^{-10} m/s (Johannesson et al., 1999), with the relationship for the unsaturated 392 393 variation of hydraulic conductivity shown in table 2 used for backfill with the value δ =10 394 found to correlate well with experimental data (Börgesson and Hernelind, 1998). 395 Experimental water-retention data presented by Börgesson and Hernelind (1999) have been 396 fitted to a van Genutchen relationship. A saturated thermal conductivity of 1.5W/m/K is employed (Börgesson and Hernelind, 1999) with a similar form of variation with water 397 398 saturation to MX-80 assumed:

$$\lambda_{T} = 0.3 \qquad S_{l} \le 0.2$$

$$\lambda_{T} = 0.3 + \frac{11}{6}(S_{l} - 0.2) \qquad 0.2 < S_{l} \le 0.8 \qquad (2)$$

$$\lambda_{T} = 1.0 + 0.5S_{l} \qquad 0.8 < S_{l} \le 1.0$$

Limited mechanical data is available for the backfill, e.g. Mata (2003), however this is for a mixture of MX-80 bentonite and rock. Oedometer experiments presented were found to give κ =0.016 and $\lambda(0)$ =0.102. Due to a lack of similar experimental evidence in suction controlled conditions the values of *M*, *r* and β will be assumed to be consistent with the MX-80. Volume changes with respect to suction change, κ_s are assumed to be governed by the clay volumetric fraction, i.e. 30%, and the coefficient of thermal expansion, α_T , consistent with the volumetric fractions of rock and clay, i.e. 30% clay and 70% rock.

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408 **4 Transient flow behaviour of bentonite**

409 **4.1 MX-80 bentonite**

410 A number of investigations of coupled THM behaviour of in-situ tests (Thomas et al 2003, 411 2009) have demonstrated a requirement to incorporate the impact of microstructural 412 behaviour within compacted bentonite barriers. In those studies an approach of 'choking' moisture flow in confined conditions on increasing saturation was found to significantly 413 414 improve the results. In this study this approach is further developed to represent the effect of 415 transient microstructural behaviour on hydraulic flow (Vardon, 2009). A number of 416 processes impacting the flow behaviour of compacted bentonite can be identified and include 417 i) time required for free and microstructure absorbed water to reach equilibrium; ii) 418 availability of free water to allow microstructural swelling; iii) ageing of manufactured 419 bentonite resulting in a reduction in the proportion of macro-pores; iv) impact of flow-rate 420 and swelling on the creation, enlargement or healing of preferential pathways for flow; and v) 421 the confinement conditions (Tang and Cui, 2005; Dueck, 2008; Delage et al., 2006; Cui et al., 422 The approach presented by Thomas et al. (2003, 2009) has been applied, via 2008).

423 numerical modelling, when flow-rates are relatively slow. In those studies instantaneous 424 equilibrium is assumed with a fixed proportion of water absorbed into the micro-pores. The 425 impact of faster in-flow rates where microstructural swelling takes place at a different time 426 scale may have not been captured using that approach. The work presented here includes a 427 methodology which more fully captures the process of microstructural swelling at the faster 428 macro flow rates.

429 **4.2 Pelletised MX-80 bentonite**

For the hydraulic conductivity of pelletised bentonite, Hoffmann et al. (2007) presented two 430 431 relationships based on fast and slow infiltration. It can be noticed that initially the inter-pellet 432 voids dominate and as the pellets expand the hydraulic conductivity is reduced; therefore the 433 rate of pellet expansion is the limiting factor. For slow infiltration the pellets are able to 434 expand as water flows and the conductivity will reduce; whilst for rapid infiltration the pellets 435 will not initially have time to expand and the conductivity will remain high until enough time 436 has passed to allow pellet expansion. A similar observation is made by Alonso et al. (2011). 437 In an attempt to capture this behaviour an initial approach is presented here to represent 438 transient change in conductivity as the pellet region hydrates based on the assumptions that i) 439 inter-pellet pores initially dominate during the saturation process, ii) an initial hydraulic 440 conductivity exists based upon the mean pellet size, pellet-size distribution and pellet 441 compaction, iii) a final hydraulic conductivity exists, based upon the final homogenised structure, iv) only monotonic wetting paths are considered, and v) above a specified degree-442 443 of-saturation the pellet region moves towards a homogenised state at a constant rate. In this 444 study an approach is utilised to represent the effect of transient behaviour on hydraulic flow 445 (Vardon, 2009), with the material relationships defined in table 2.

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447 To investigate the proposed model of the pelletised MX-80 a series of analyses of the 448 Cannister Retrieval Test has been undertaken (Vardon, 2009). From these tests a set of 449 calibrated parameters for the pelletised region have been obtained $(k_{init}=1\times10^{-10}m/s)$, 450 $k_{inf}=1\times10^{-16} m/s$, $\beta_p=1\times10^{-7} s^{-1}$, and $S_{lA}=0.3$). In the absence of experimental data, the 451 moisture-retention curve for compacted MX-80 has been adopted.

452

453 **5 Simulations**

454 **5.1 Pre-Placement Simulation**

The simulation performed includes all the identified hydraulic features identified in section 2, including the region of high hydraulic conductivity (*Region 1*). The hydraulic conductivities are based upon the transmissivities quoted by Rhén and Forsmark (2001), or the central figure when a range is quoted. The analysis was run for 2 years, at which point a pseudo steady-state had been achieved, where the rate of change in inflow into the deposition-holes and tunnel system is found to be less than 1%. The mesh has been checked for spatial convergence and the time step for temporal convergence.

462 **5.1.1 Initial and boundary conditions**

463 The reported inflow rates, shown in figure 3(a) and 3(b), show little variation over the time 464 they were recorded (Rhén and Forsmark, 2001). Although the construction of the tunnel was 465 undertaken over time, the initial conditions for this simulation were assumed to be hydrostatic 466 with the mean sea level. Boundary conditions on the far field have been maintained at 467 hydrostatic pore-water pressure. The distance the boundary is set from the repository has been found not to affect the results through monitoring of the boundary fluxes. On the 468 469 interior of the tunnel and deposition-holes, following the approach of Thomas et al. (2009), 470 the pore-water pressure has been fixed at zero to reflect the atmospheric pressure. This was 471 also found experimentally, e.g. Mishra et al. (2008).

472 **5.2 Post-Placement Simulations**

473 **5.2.1 Boundary conditions and initial condition**

474 On the outer boundaries the temperature is fixed at the initial value, the pore-water pressure is 475 fixed at hydrostatic pore-water pressure with the exception of the far boundary which the 476 tunnel intersects, where a zero moisture flux boundary condition was applied. The deformation domain is fixed normal to the boundary at the outer edge. At the boundary of the canister/buffer interface, a zero moisture flux condition was applied with deformation normal to the canister surface restrained. A heat flux was applied on the surface of the canister based upon the total energy provided to the heater. Initially the temperature is set to 289*K* throughout the domain, based upon initial experimental evidence. The stress conditions in the rock mass as recorded and resolved in coordinates orthogonal to the repository are:

$$\begin{cases} \sigma_{x} \\ \sigma_{y} \\ \sigma_{z} \\ \tau_{z} \\ \tau_{yz} \\ \tau_{zx} \\ \tau_{$$

484 where x is along the tunnel length, y is vertical and z is perpendicular to both x and y. The initial pore-water pressure in the buffer and backfill material was based upon the water 485 486 content and degree of saturation reported from installation measurements by Börgesson et al. 487 (2002) and Johannesson et al. (2004) and the retention properties presented in table 2. The 488 compacted bentonite cylinders and rings were found to have an initial pore-water pressure of 489 -64.7 and -49.2MPa respectively (based upon degrees of saturation of 0.79 and 0.86 490 respectively), with the bricks and pellets -112 and -111MPa (degrees of saturation of 0.64 491 and 0.25 respectively).

492

483

493 **6 Results**

A single simulation has been undertaken for the pre-placement phase, where the proposed model inclusive of deterministic features has been implemented. Data from the simulations is compared with the salient experimental evidence, namely the inflow rate along the repository tunnel, shown in figure 3(a), the inflow rates in the deposition-holes, shown in figure 3(b) and a contour plot of the pore-water pressure along the centre-line is shown in figure 8. This analysis can be seen, by consideration of figure 3(a), to simulate the inflow into the tunnel 500 closely. Importantly there is good qualitative trends displayed, with a great difference in 501 inflow rate at chainages above and below 3 588m. Considering the flow into the deposition-502 holes, seen in figure 3(b), this analysis is able to simulate the flows into DHs 2-6, with the numerical results following the experimental results closely. The simulated inflow into DH-1 503 504 is approximately only 12% of the experimental value, however it is significantly higher than 505 that simulated for DHs 2-6 showing a trend that is in agreement with the experimental results. 506 Simulation of the inflow into DH-1 could be quantitatively improved by altering the 507 hydraulic conductivities in the model, however such a modification would require a priori 508 knowledge of the inflows; also this does not guarantee that this is the correct mechanism. For 509 example, the same result could also be achieved by increasing the size of the closest fracture; 510 therefore the parameters derived from experimental data have continued to be used.

511

Figure 8, highlights the effects of the major features. The edge of the major fracture, indicated in the figure, can be seen between DH-1 and the end of the tunnel. The effect of this feature can be seen by the extended contour of approximately 1MPa, extending vertically from the repository tunnel.

516

517 Results for the initial operational phase of the post-placement analysis, i.e. up to 10 years, are 518 presented in figures 6, 7 and 9-12, when the thermal and hydraulic gradients are at their 519 greatest, due to the greatest heat output from the canisters and the initially unsaturated state of 520 the bentonite. In this time the peak temperature is likely to be found, as the heat output is the 521 greatest, and therefore the moisture regime will be greatly influenced by the heat distribution. 522 The post-placement results are presented at mid-height of the buffer, although they have also 523 been compared in other locations. The temperature results for DH-1 and DH-3 are shown in figures 6(a) and 7(a), with the numerical results correlating well with the experimental 524 525 results. Examining the temperature contour plot shown in figure 9, the temperature fields 526 from the deposition-holes can be seen to 'interact' increasing the temperature, demonstrating

527 that a three-dimensional analysis is essential. Consequently, the temperature exhibited by 528 DH-3 is higher than that of DH-1, as expected by its position in the PRP. The relative 529 humidity results for DH-1 and DH-3 are shown in figures 6(b) and 7(b). In DH-1, it is seen that the numerical results simulate the experimental behaviour well. It is noted that the effect 530 531 of the fracture seen in the contour plots in figure 10 creates a large spatial gradient and the 532 results are therefore sensitive to the exact sensor location and subtleties of the 533 fracture/deposition-hole interaction. A possibly significant difference is that the inner-most 534 sensor location, sensor WBU10013 at 0.585m radius, does not saturate as quickly as shown 535 experimentally and therefore allows vapour transport to continue. It is not clear if this 536 location is saturated experimentally as the sensor has stopped working. Significantly for long 537 term simulations, the gradients of re-saturation shown in the simulations are almost identical 538 to that shown by all the sensors experimentally when they fail or at the final recording. In 539 figure 7(b) the numerical results correlate well to the experimental results, with a slight overestimation of re-hydration, but exhibiting good qualitative trends. The final gradients 540 541 shown experimentally are also reproduced well in the simulation. Figures 6(c) and 7(c) present the mechanical evolution in terms of net mean stress for both experimental and 542 543 numerical results. The numerical results are reasonable in stress magnitude and importantly, 544 differences in magnitudes correlate well with experimental results. The results also correlate 545 with the hydraulic behaviour, that is, where significant hydration has occurred stresses due to swelling have occurred. The increase in stresses noted after approximately 2,000 days is due 546 547 to the increase in saturation shown by the model at this point, which is driven by a reduction in heat output from the canisters. 548

549

Figures 9-11 present contour plots at vertical cross-sections through the centre-line of the tunnel for the temperature, pore-water pressure and displacement. Figure 9 shows the thermal interaction between the DHs and shows the transient thermal behaviour as well as a power failure in DH-2. It can be seen in figure 10 that the backfill largely saturates over the 554 first 2,500 days, which is in agreement with the experimental results (Goudarzi and 555 Johannesson, 2007). The backfill behaves as a relatively large water sink in this period. It 556 can also be seen that the resaturation behaviour in DH-1 is local to the fracture and that at the top and the bottom of the buffer the qualitative trend is similar to that of DH-3, as exhibited 557 558 experimentally. In figure 11 the displacement results indicate that the swelling in the 559 compacted buffer will cause lateral movement towards the pellets, as expected, and also a 560 displacement towards the tunnel into the backfill material. This displacement, however, does 561 not cause the buffer material to penetrate the tunnel. Figure 12 shows a pore-water pressure 562 contour-plot on a horizontal cross-section through the tunnel, highlighting the impact of the major fractures on the pore-pressure surrounding the tunnel. 563

564

565 7 Discussion

The model results illustrate that the early stage (e.g. 5 years) the thermo-hydro-mechanical 566 behaviour can be well reproduced. This gives confidence that such models can be utilised in 567 568 safety assessment. Longer term behaviour, such as extrapolation to hundreds of years is less certain. Therefore long-term experimentation remains extremely valuable. It is noted that 569 570 the model relies on accurate and detailed geological characterisation and that the accurate 571 performance of the system cannot be modelled using two-dimensional or averaged material parameters. A model such as this could be further utilised to give a proportion of behaviour, 572 573 in terms of, for example, the number of deposition-holes having a certain 574 saturation/temperature/stress, which may therefore give an indication of system performance in terms of reliability. 575

576 Such an early stage (pre-saturation) model is useful as it is during this time that heat output is 577 highest, and also thermal conductivity is the lowest, therefore design limits based on 578 temperature will require such models, so as not to be overly conservative. Furthermore the 579 recent development of THM models to include consideration of chemical species (e.g. Cleall 580 et al., 2007; Gens, 2010) and the impact of advective processes on the geochemical

581 conditions close to the canister (Thomas et al., 2012; Cleall et al., 2013; Masum et al., 2013) 582 and the potential for enhanced corrosion and gas production highlights the need for 583 confidence in the correct representation of moisture and gas movement in the short-term near field behaviour of repository systems. It is noted that the model requires a large number of 584 585 material parameters to be determined. However, a large proportion are for the expansive 586 clay, which is part of the engineered barrier. This means that material variability is able to be 587 controlled and is likely to be low, therefore these do not pose an undue burden on the operator of such a programme. The parameters for the rock are significantly fewer with the 588 589 permeability being one of the most variable and also influential, as it is from here that water 590 is supplied to the buffer/backfill material.

591

592 8 Conclusions

A model of the prototype repository system has been presented, based upon a fully threedimensional finite-element formulation. This allows for the inclusion of inherent anisotropy due to the existence of fractures. In particular the local influences of known fractures are included. The pre-placement stage has first been modelled, where large variations in inflow rate have been captured. It has been demonstrated that the hydraulic performance is inherently three-dimensional and should be modelled as such to gain meaningful results.

599 A three-dimensional Thermo/Hydro-/Mechanical (THM) investigation is then presented. The 600 key aspects of the THM behaviour of the repository are well captured by the modelling 601 strategy, namely: i) three-dimensional behaviour in the thermal, hydraulic and mechanical fields; ii) close correlation of numerical result of the thermal field with experimental values; 602 603 iii) backfill hydration similar to that reported experimentally; iv) drying of buffer material 604 close to heaters and wetting adjacent to rock reproduced; v) anisotropic hydration behaviour reproduced; and vi) swelling pressure increases with hydration, with differences in 605 606 magnitudes represented. The temperature field was noted to be intrinsically three-607 dimensional, with the effects of adjacent canisters' heat output influencing the temperature

within other deposition-holes. The hydraulic importance of the fracture intersecting DH-1 was highlighted and the highly three-dimensional anisotropic hydration behaviour noted and reproduced. The significance of the backfill as a substantial sink for pore-water was demonstrated with the simulations able to largely reproduce the saturation time exhibited experimentally with the geological supply of water was critical to the hydration rate of various aspects of the repository.

614

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730 List of tables

- 731 Table 1. Preliminary fracture model data, including initial hydraulic conductivity estimates
- for the fractures, items marked * after Rhén and Forsmark (2001).
- 733 Table 2. Material parameters.
- 734

735 List of figures

- Figure 1. Schematic of the PRP project (after Svemar and Pusch, 2000).
- Figure 2. Materials contained within the repository.

Figure 3. Tunnel and deposition-hole inflow measurements. a) Experimental data for the tunnel inflow (after Rhén and Forsmark, 2001) and the numerical results; b) Experimental data for the inflow into the deposition-holes (after Rhén and Forsmark, 2001) and the numerical results.

- Figure 4. Fracture map of along the tunnel, where the centreline is the roof (after Rhén and
 Forsmark, 2001). Water bearing structures are identified throughout as circles and two areas
 of large inflows are highlighted as '*Area 1*' and '*Area 2*'.
- Figure 5. Visualisations of the model domain. a) complete domain; b) view from above therepository tunnel c) detailed view of DH-5 and 6 d) DH-1 to 3.
- Figure 6. Numerical and experimental results for temperature, relative humidity and net mean
 stress measurements at mid-height in DH-1. Experimental results after Goudarzi and
 Johannesson (2007).
- Figure 7. Numerical and experimental results for temperature, relative humidity and net mean
 stress measurements at mid-height in DH-3. Experimental results after Goudarzi and
 Johannesson (2007).

Figure 8. Contour plot of results from pre-placement analysis complete with discretefractures in the model domain.

- 755 Figure 9. Contour plots of temperature (*K*) variation in the simulation.
- Figure 10. Contour plots of pore-water pressure (*Pa*) variation in the simulation (DH-1 toDH-4).
- 758 Figure 11. Contour plots of displacement (*m*) variation in the simulation (DH-1 to DH-4).
- 759 Figure 12. Contour plots of pore-water pressure (Pa) variation in the simulation in a
- 760 horizontal cross section intersecting the tunnel.

Table 1. Preliminary fracture model data, including initial hydraulic conductivity estimates

for the fractures, items marked * after Rhén and Forsmark (2001).

Feature	East*	North*	\mathbf{Z}^*	Strike*	Dip*	Radius*	\mathbf{Tr}^*	Thickness ^b	Hydraulic Conductivity ^c , K_{feat}	Analysis Hydraulic Conductivity, K_{feat} (m/s)
	(<i>m</i>)	(<i>m</i>)	(mamsi)	()	()	(<i>m</i>)	(m /s)	(<i>m</i>)	(11/3)	(11/3)
Intact rock										$1.0 imes 10^{-11}$
Major features										
North Major*	1 892	7 289	-449	118	88	20	$5 10 imes 10^{-8}$	0.1	$5 - 10 \times 10^{-7}$	$8 imes 10^{-7}$
South Major*	1 887	7266	-449	124	89	20	$7-9 imes 10^{-8}$	0.1	$7-9 imes 10^{-7}$	$8 imes 10^{-7}$
Region 1										8 x 10 ⁻⁷
Minor features										
3587/1*	1 878.28	7 275.03	-453.53	354	79	2	$8.1 imes 10^{-9}$	0.05	1.62×10^{-7}	$1.6 imes 10^{-7}$
3551/1*	1 915.42	7 271.06	-455.24	312	40	2	$4.7 imes 10^{-9}$	0.05	$9.4 imes 10^{-8}$	$9.4 imes 10^{-8}$
3551/2*	1 917.50	7 269.90	-455.56	271	38	2	$3.3 imes 10^{-9}$	0.05	$6.6 imes 10^{-8}$	$6.6 imes 10^{-8}$
3545/1*	1 919.55	7 268.80	-453.54	164	64	2	2.8×10^{10}	0.05	$5.6 imes 10^{-9}$	$5.6\times 10^{\text{-9}}$
3545/2*	1 919.55	7 268.80	-456.66	278	24	2	1.7×10^{-9}	0.05	$3.4 imes 10^{-8}$	$3.4 imes 10^{-8}$
3545/3*	1 921.45	7 270.22	-453.14	298	64	2	$1.3\times 10^{\text{-8}}$	0.05	$2.6 imes 10^{-7}$	$2.6 imes 10^{-7}$

^ametres above mean sea level, ^bassumed, ^cderived *East, North and Z are all coordinates in the Äspö coordinate system and Tr is the transmissivity.

Properties	Rock	Fractures	MX-80 buffer	MX-80 pellets	Backfill	Concrete
Porosity, n	0.005	0.1	0.4 cylinders, 0.36 rings, 0.384 bricks	0.61	0.363	0.005
$\rho_s (\text{kg/m}^3)$	2770	2770	2780	2780	2780	2770
Heat capacity of solid, <i>C</i> _{ps}	750	750	800	800	850	750
$\lambda_T (W/mK)$	2.5	2.5	0.3-1.3 as equation 1	0.3-1.3 as equation 1	0.3-1.5 as equation 2	2.5
<i>K</i> _l (m/s)	$K_{l} = K_{sat} S_{l}^{0.5} (1 - (1 - S_{l}^{j/\beta_{l}})^{\beta_{l}})^{2}$	As rock	$K_{swell} = K_{sal} (S_l)^{\delta} (1 - \omega_{abs} S_l)$ $\frac{\partial \omega_{abs}}{\partial t} = \alpha - \frac{S_{tabs}}{S_l^2} \frac{\partial S_l}{\partial t}$ where $\omega_{s} \leq \omega^{max}$ and $S_l < 1$	$\begin{split} K_{pel} = (1 - \omega_{pel}) k_{init} + k_{inf} \omega_{pel} \\ \frac{\partial \omega_{pel}}{\partial t} = \beta_p \end{split}$	$K_l = K_{sat} S_l^{\delta}$	As rock
Constants	$K_{sat} = 5.0 \times 10^{-12}$	$K_{sat} =$ various	$K_{sat} = 1.9 \times 10^{-14}$	$k_{init} = 1.0 \times 10^{-10}$	$K_{sat} = 1.5 \times 10^{-10}$	$\begin{array}{l} K_{sat} = \\ 1.0 \times 10^{-14} \end{array}$
			$\alpha_l = 1.0 \times 10^{-7}$ $\delta = 3$	$k_{inf} = 1.0 imes 10^{-16} \ eta_p = 1.0 imes 10^{-7}$	$\delta = 10$	
S_l	$S_{l} = \left(1 + \left[\frac{s}{P_{0}}\right]^{l_{l-\beta_{l}}}\right)^{-\beta_{l}}$	As rock	$nS_{l} = \theta_{res} + \frac{\theta_{sal} - \theta_{res}}{\left(1 + \left[\frac{1000\alpha s}{\rho_{l}g}\right]^{b}\right)^{\left(1 - \frac{1}{b}\right)}}$	As MX-80 buffer	As MX-80 buffer	As rock
Constants	$\beta = 0.33$ $\beta = 0.33$		$\alpha = 1.25 \times 10^{-7} (m^{-1})$	$\alpha = 7.00 \times 10^{-6}$	$\alpha = 1.00 \times 10^{-4}$	$\beta = 0.33$
	$P_0 = 0.33 (\text{Pa}^{-1})$	$P_0 = 0.33$	b = 1.75	<i>b</i> = 1.30	<i>b</i> = 1.23	$P_0 = 0.33$
			$\theta_{res} = 0.0001$	$\theta_{res} = 0.0001$	$\theta_{res} = 0.0001$	
			$\theta_{sat} = n$	$\theta_{sat} = n$	$\theta_{sat} = n$	
	Initial condition, $S_l = I$		Initial conditions (cylinders, rings, bricks), $S_l=0.79$, 0.86,0.64	Initial condition, $S_l = 0.25$	Initial condition, $S_l = 0.524$	Initial condition, $S_l=1$
G (MPa)	27600	27600	10	1	10	27600
υ	0.25	0.25	-	-	-	0.25
κ	-	-	0.0245	0.25	0.016	-
λ(0)	-	-	0.238	0.6	0.102	-
p_c (MPa)			$1.0 imes 10^5$	1.0×10^{5}	1.0×10^{5}	-
p_0^* (MPa)	-	-	45	45	45	-
β	-	-	1.0	1.0	1.0	-
r	-	-	0.9	0.9	0.9	-
М	-	-	0.358	0.358	0.358	-
k	-	-	5.6×10^{-3}	5.6×10^{-3}	$1.7 imes 10^{-3}$	-
\mathcal{K}_{S}	-	-	0.075	0.075	0.025	-
$\alpha_T(\mathbf{K}^{-1})$	$8.0 imes10^{-6}$	$8.0\times10^{\text{-6}}$	$1.0 imes10^{-4}$	$1.0 imes 10^{-4}$	$3.56\times 10^{\text{-5}}$	$8.0\times10^{\text{-6}}$





Figure 1. Schematic of the PRP project (after Svemar and Pusch, 2000).



Figure 2. Materials contained within the repository.



Figure 2. Materials contained within the repository.



Figure 3. Tunnel and deposition-hole inflow measurements. a) Experimental data for the tunnel inflow (after Rhén and Forsmark, 2001) and the numerical results; b) Experimental data for the inflow into the deposition-holes (after Rhén and Forsmark, 2001) and the numerical results.

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Figure 4. Fracture map of along the tunnel, where the centreline is the roof (after Rhén and Forsmark, 2001). Water bearing structures are identified throughout as circles and two areas of large inflows are highlighted as 'Area 1' and 'Area 2'.

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Figure 5. Visualisations of the model domain. a) complete domain; b) view from above the repository tunnel c) detailed view of DH-5 and 6 d) DH-1 to 3.

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Figure 6. Numerical and experimental results for temperature, relative humidity and net mean stress measurements at mid-height in DH-1. Experimental results after Goudarzi and Johannesson (2007).

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net mean stress measurements at mid-height in DH-1. Experimental results after
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Figure 7. Numerical and experimental results for temperature, relative humidity and net mean stress measurements at mid-height in DH-3. Experimental results after Goudarzi and Johannesson (2007).

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Figure 7. Numerical and experimental results for temperature, relative humidity and
net mean stress measurements at mid-height in DH-3. Experimental results after
Goudarzi and Johannesson (2007).



Figure 8. Contour plot of results from pre-placement analysis complete with discrete fractures in the model domain.

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- 801 fractures in the model domain.

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Figure 9. Contour plots of temperature (K) variation in the simulation.

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Figure 9. Contour plots of temperature (*K*) variation in the simulation.



Figure 10. Contour plots of pore-water pressure (Pa) variation in the simulation (DH-1 to DH-4).

- 807 Figure 10. Contour plots of pore-water pressure (Pa) variation in the simulation (DH-
- 808 1 to DH-4).



Figure 11. Contour plots of displacement (m) variation in the simulation (DH-1 to DH-4).

811 Figure 11. Contour plots of displacement (m) variation in the simulation (DH-1 to

812 DH-4).



Figure 12. Contour plots of pore-water pressure (*Pa*) variation in the simulation in a horizontal cross section intersecting the tunnel.

- 815 Figure 12. Contour plots of pore-water pressure (Pa) variation in the simulation in a
- 816 horizontal cross section intersecting the tunnel.
- 817