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Äspö Hard Rock Laboratory

Prototype Repository

Predictive modelling of EBS preformance in the Prototype Repository Project

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March 2003

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PROTOTYPE REPOSITORY

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Abstract

The present report summarizes attempts to predict the most important processes in the evolution of the buffer and backfill by applying THMCB models for later comparison with data recorded by use of the comprehensive instrumentation of the Prototype Repository. The basic input to the calculations is the material properties of the buffer and backfill originally given by SKB, and a conceptual model of expected processes involved in the evolution of the EBS components buffer and backfill. Boundary conditions in terms of the piezometric and other hydraulic conditions in the nearfield rock have been specified since they are necessary prerequisites for the calculations.

The report contains a brief summary of the various THMCB codes used for predicting the evolution of the EBS, focusing on the buffer and backfill but including also canister movement and chemical changes in the porewater.

The final part of the report gives examples of the outcome of predictive calculations of major processes, particularly the temperature changes and the wetting of the buffer and associated strain of the buffer.

Sammanfattning

Rapporten ger en sammanfattning av försök att förutsäga viktiga processer i utvecklingen av buffert och återfyllning genom användning av THMCB-modeller för senare jämförelse med data erhållna från den omfattande instrumenteringen av Prototypförvaret. Grunden för beräkningarna utgörs av materialdata som urspungligen gavs av SKB och av en konceptuell modell för förväntade processer i buffertens och backfillens utveckling. Gränsvillkoren uttryckta i form av piezometerdata och andra hydrauliska förhållanden i närfältet har specificerats eftersom de utgör nödvändiga förutsättningar för beräkningarna.

Rapporten innehåller en kort summering av de olika THMCB-koderna som används för predikteringen av utvecklingen av EBS med fokus på bufferten och återfyllningen men omfattande också kanisterrörelser och kemiska förändringar hos porvattnet.

Rapporten avslutas med att ge exempel på utfallet av predikteringar av viktiga processer, särskilt temperaturändringar och bevätning och därav orsakade deformationer hos bufferten.

Contents

1 Introduction

1.1 General

The Prototype Repository Project aims at collecting information and experience in designing and constructing repositories in crystalline rock, to work out and test thermo-hydro-mechanical-chemical-biological (THMCB) models for predicting and evaluating the function of such repositories. The major objectives of the project are:

- To simulate part of a future KBS-3 Deep Repository to the extent possible with respect to geometry, materials and rock environment except that radioactive waste is simulated by electrical heaters. Figure 1 is a longitudinal section through the test drift indicating the instrumentation used for prividing data for assessing the relevance and accuracy of the theoretical models. The comprehensive instrumentation of some of the deposition holes is not shown (cf. Table 1.).

- To test and demonstrate the integrated function of repository components and to compare results with predictive calculations based on conceptual and theoretical models.

- To develop, and test appropriate engineering standards and quality assurance methods.

- To simulate appropriate parts of the repository design and construction processes.

The present report summarizes attempts to predict the most important processes in the evolution of the buffer and backfill by applying THMCB models for later comparison with data recorded by use of the instrumentation summarized in Figure 1 and Table 1.

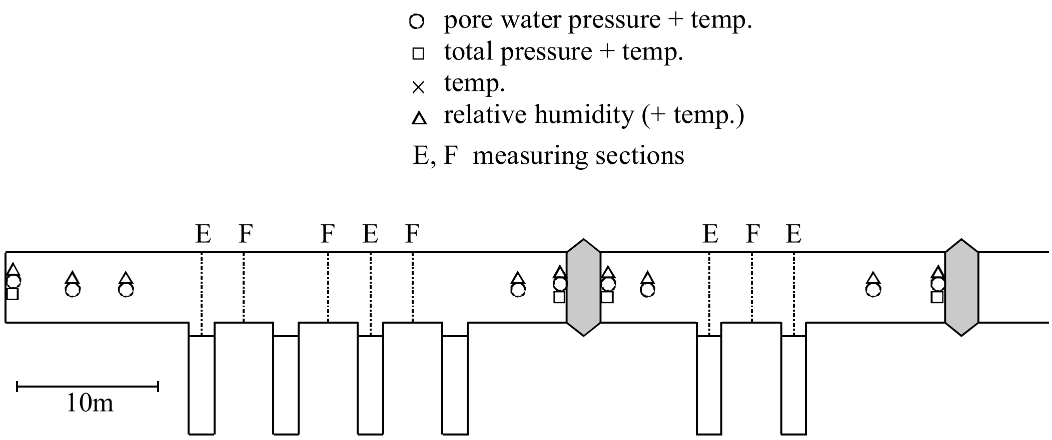


Figure 1. *The Prototype Repository test drift with instrumentation of the tunnel backfill. Only four of the six deposition holes are instrumented, i.e. the 1st and 3rd holes in the left section and the two holes in the right section.*

Table 1. Measuring principles for the Prototype Repository [1].

Measuring quantity	Measuring principle	Number of sensors in section I		Number of sensors in section II		Total number
		Tunnel	Deposition hole	Tunnel	Deposition hole	
Temperature	Thermocouple	20	64	16	64	164
	Fibre optic (DTS/FTR)	0	8	0	4	12
Total pressure	Vibrating wire	10	28	8	28	74
	Piezoresistive	10	28	8	28	74
Pore water pressure	Vibrating wire	12	14	10	14	50
	Piezoresistive	12	14	10	14	50
Water content	Relative humidity (capacitive method)	0	74	0	74	148
	Soil Psychrometry	45	0	32	0	77
Porewater chemistry	Tubes for sampling				10	?
Total		109	230	84	226	649

The work is performed under the following subpackages:

- WP3a Water and gas sampling and analysis
- WP3b Hydraulic tests in rock
- WP3c THM Laboratory tests on buffer and backfill properties
- WP3d Laboratory tests on mechanical properties of rock
- WP3e Laboratory determination of cracks in EDZ
- WP3f T and TM modelling (rock)
- WP3g HM and THM modelling of rock
- WP3h THM modelling of buffer, backfill and interaction with near-field rock
- WP3i C modelling of buffer, backfill and groundwater

In this report focus is on WP3h and WP3i, which deal with predictive modelling of the evolution of the buffer and backfill.

1.2 Conditions

Prediction of all important processes in the evolution of the buffer and backfill by use of the theoretical THM models requires three major types of information:

1. Material data - buffer, backfill, canister, rock.
2. Conceptual model - description of processes that are involved in the evolution of the buffer and backfill.
3. Boundary conditions - rock structure (fractures, EDZ, access to water at the buffer/rock contact, rock water pressure)

1.2.1 Material data (original)

The data needed for predicting the evolution of the buffer and backfill are collected in [2].

1.2.2 Conceptual model

The following changes will occur in the system of highly compacted smectitic blocks (MX-80) confined by the overlying backfill and the surrounding rock as indicated in Figure 2:

1. Thermally induced redistribution of the initial porewater.
2. Maturation of the 50 mm thick pellet backfill, implying homogenisation and consolidation of this buffer component under the swelling pressure exerted by the hydrating and expanding blocks.
3. Uptake of water from the rock and backfill leading to hydration of the buffer.
4. Expansion of the buffer yielding displacement of the canisters and overlying backfill.
5. Penetration of buffer into open fractures in the rock.
6. Dissolution of buffer minerals and precipitation of chemical compounds in the buffer.

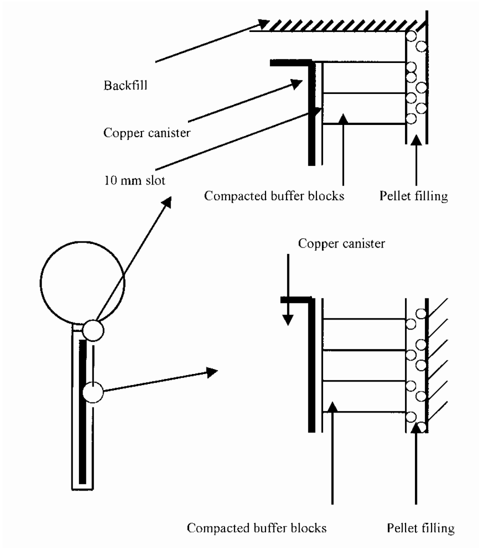


Figure 2. *KBS-3 deposition hole with copper-shielded canister embedded in compacted buffer blocks and bentonite pellet filling.*

The various processes are coupled in a complex way and cause transient changes in the material properties. This makes the modelling difficult and requires a number of simplifications, one being that the soil is taken to be a homogeneous medium although it is in fact strongly heterogeneous with water vapour and water moving in different types of voids.

The pellets in the 50 mm water-filled gap offer difficulties in the modelling. They disintegrate quickly and form a rather soft clay gel from which water is sucked by the very dense clay blocks which thereby expand and consolidate the gel to become as dense as the expanded blocks. The process has a B-effect implying that microbes can enter the pellet filling and survive and multiply until the density of the filling has approached 1600 kg/m^3. The transient conditions are exemplified as follows:

- Buffer penetrating into water-bearing fractures with an operator of more than about 140 µm will seal the fractures and force inflowing water to follow other less wet parths.
- The hydraulic conductivity of the outermost part of the buffer - the pelletfill- drops and the inflow of water from the rock into the deposition holes decreases.
- There is competition with respect to water between the densifying pellet filling and the softening buffer blocks.
- The consolidated clay gel formed by the hydrated and expanded pellets, becomes anisotropic from the initial isotropic state due to the vertical particle orientation induced by the high horizontal pressure.

1.2.3 Boundary conditions

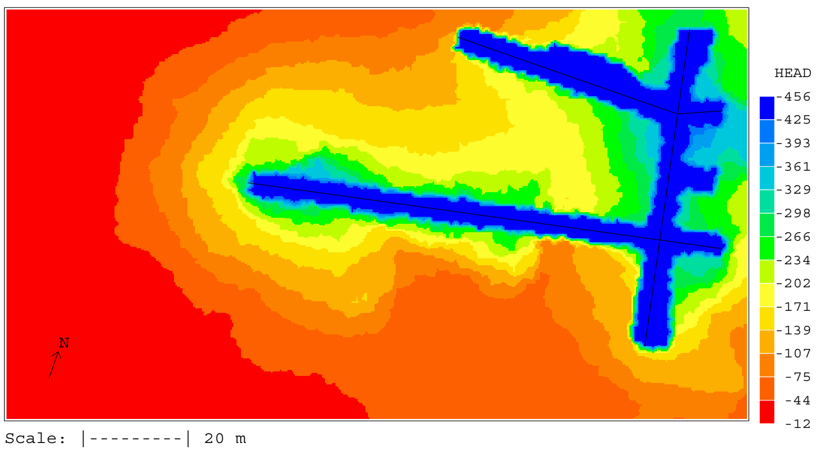
Uptake of water from the rock is the THMC process that ultimately yields complete water saturation and the final density distribution. If the rock gives off very little water to the deposition holes the backfill may serve as the major water source. The water transport from the backfill to the buffer is controlled by the water pressure and by the suction of the buffer, as well as by the degree of water saturation of the backfill. The water pressure in the permeable backfill may rise relatively quickly if it is supplied with water from intersected fracture zones but may otherwise be rather low.

The hydraulic transport capacity of the rock surrounding the deposition holes depends on the frequency and conductive properties of the discontinuities, while the distribution over the periphery of the holes is controlled both by the location of intersecting hydraulically active fractures and by the conductivity of the shallow boring-disturbed zone (EDZ). The three most important parameters to be used in applying the THM-models are 1) the piezometric pressure in the near-field rock, 2) the frequency of hydraulically active fractures that can bring water to the deposition holes yielding the average hydraulic conductivity of the near-field rock, and 3) the hydraulic conductivity of the EDZ.

Hydraulic conditions

Pressure and temperature conditions in the rock at the start of the evolution of the buffer and backfill form the basis of the various THMCB modelling attempts and data made available in the course of the project can be used for calibration and updating of the models [3].

The water pressure at about 2 m distance from the tunnel wall is between 100 kPa and 1.5 MPa. Varying the hydraulic conductivity of the backfill from E-11 to E-9 to m/s gave corresponding water pressure distributions in the rock. Figure 3 shows the distribution of pressure and salinity at the level where the field test is conducted.



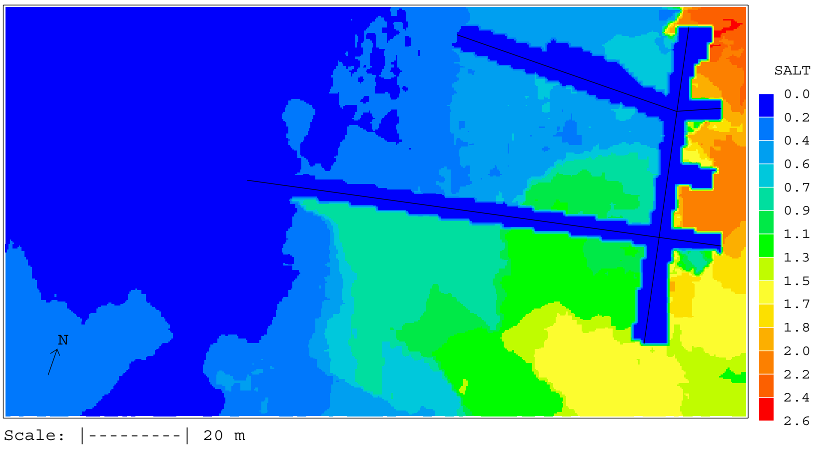
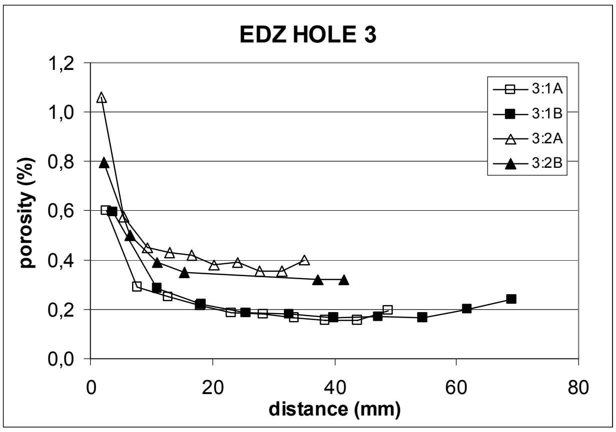


Figure 3. *Pressure head (m) in the upper figure and salinity (%) at 447 m depth [Rhen et al].*

The average bulk hydraulic conductivity of the near-field rock around the deposition holes is K=E-12 to K = 4E-10 m/s. Using rock structure data a deposition hole is expected to be intersected by about 3 steep and 4 flat lying, significantly water-bearing fractures, which somewhat overrates the actual numbers. The average inflow of water in the holes is less than 0.006 l/min in all the holes except Hole 1, which has an inflow of 0.08 l/min.

In situ measurement of the EDZ by BGR has been made in the access tunnel immediately in front of the Prototype Repository test site, showing that the hydraulic conductivity within about 10 cm distance from the tunnel wall is higher than of the rock matrix further off from the wall. Within 1 cm depth the conductivity was found to be about E-10 m/s, while it was estimated at E-12 to E-10 m/s from 1 to 10 cm depth.

A POSIVA study by impregnation of ^{14}C-polymethylmethacrylate (^{14}C-PMMA) for scanning electron microscopy (SEM) confirmed BGR's findings (Figure 4). Thus, a 10-20 mm disturbed zone had a higher porosity than undisturbed rock and the first few millimetres were significantly more porous as demonstrated earlier by a study made by Geodevelopment AB.



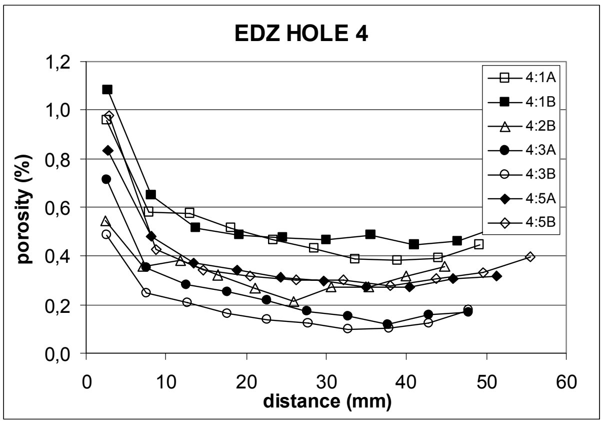


Figure 4. *Porosity of rock with respect to the distance from the surface of the deposition holes No 3 and 4 in the Prototype Repository tunnel at Äspö Hard Rock Laboratory [POSIVA].*

1.2.4 Material data (complementary)

A number of material data have been derived from laboratory tests that were conducted parallel to the field experiment. They are complementary to the ones originally recommended by SKB (section 1.2.1) and are taken as a basis of some of the modelling work. Examples of such investigations are the tests on backfill of 30 % bentonite and 70 % crushed granite (or sand) performed by CIMNE. The most important findings were that the stress/strain properties of the material are not affected by the salt concentration of the water used for saturation, while the hydraulic conductivity is strongly dependent on the salt content especially for low densities (Figure 5).

Comprehensive work of several of the Participants in the project has been made for determining the water retention potential of the buffer and backfill. This is exemplified by CIMNE's study of 30/70 bentonite-sand mixtures (Figure 6). Several discussions among them show that there is still not complete understanding of the physical background of the retention potential and different data are used by different investigators.

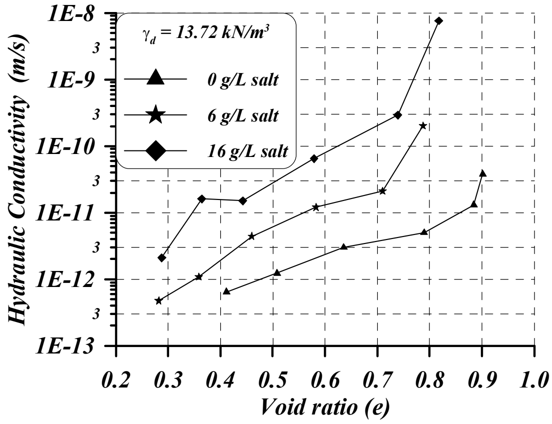


Figure 5. *Estimated hydraulic conductivities for the lowest dry density (CIMNE).*

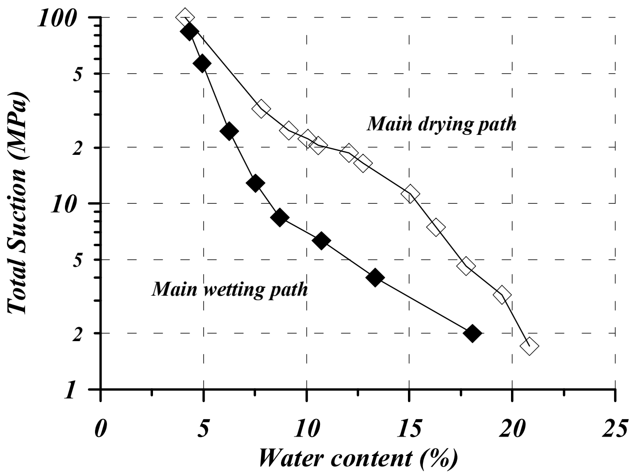


Figure 6. *Main drying and wetting retention curve for a 30/70 bentonite-sand mixture (CIMNE).*

2 Predictive Modelling

2.1 Measurements forming the basis for validation of models

The processes recorded in the Prototype Repository Project and predicted by use of theoretical models are: 1) Thermal evolution in the buffer and backfill, 2) Development of porewater pressure and water pressure in the nearfield rock, 3) Redistribution of initial porewater in the buffer and uptake of additional water, 4) Development of swelling pressure, 5) Expansion of the buffer yielding displacement of the canisters and overlying backfill, 6) Dissolution of minerals and precipitation of chemical compounds in the buffer, 7) Changes in water chemistry and microbiology.

The measurements will give information on all the important processes involved in the maturation of the buffer and backfill. Prediction of the processes by use of the models will illustrate their relevance and accuracy. They can be improved and calibrated by use of the recordings.

2.2 Summary of theoretical models

Condensed versions of proposed EBS model codes are given below [4]. Complete mathematical expressions are given in Deliverable D33 of the Prototype Repository Project.

COMPASS *(H.R Thomas and P.J Cleall, Cardiff University)*

Partly saturated soil is considered as a three-phase porous medium consisting of solids, liquid and gas. The liquid phase is considered to be pore water containing multiple chemical solutes. The gas phase is air in the pores. A set of coupled governing differential equations have been developed to describe the flow and deformation behaviour of the soil.

The main features of the formulation are:

- Moisture flow considers the flow of liquid and vapour. Liquid flow is assumed to be described by a generalised Darcy’s Law. Vapour transfer is represented by a modified Philip and de Vries approach.
- Heat transfer includes conduction, convection and latent heat of vaporisation transfer in the vapour phase.
- Flow of dry air due to the bulk flow of air arising from an air pressure gradient and dissolved air in the liquid phase are considered. The bulk flow of air is again represented by the use of a generalised Darcy’s Law. Henry’s Law is employed to calculate the quantity of dissolved air and its flow is coupled to the flow of pore liquid.

- Deformation effects are included via either a non-linear elastic, state surface approach or an elasto-plastic formulation. In both cases deformation is taken to be dependent on suction, stress and temperature changes.
- Chemical solute transport for multi-chemical species includes diffusion dispersion and accumulation from reactions due to the sorption process.

Basis for formulation of governing equations

Heat conduction and flow are expressed using classical physics but is generalized by including the velocities of liquid, vapour and air, respectively. For unsaturated soil the heat capacities of solid particles, liquid, vapour and dry air are considered in addition to the degree of saturation with respect to liquid water.

The velocities of pore liquid and pore air are calculated using a generalised Darcy's law with special respect to the chemical solute concentration gradient and the conductivity of the air phase and the pore air pressure. Also, an osmotic flow term in the liquid velocity is included for representation of liquid flow behaviour found in some highly compacted clays.

Air in partly saturated soil is considered to exist in two forms: bulk air and dissolved air. In this approach the proportion of dry air in the pore liquid is defined using Henry's law.

Where a chemical solute is considered non-reactive and sorption onto the soil surface is ignored, the governing equation for chemical transfer can be expressed in terms of diffusion and dispersion, as derived in primary variable form. The approach has been extended to a multi-chemical species form with a sink term introduced to account for mass accumulation from reactions due to the sorption process. This is then coupled to a geochemical model.

The total strain, ε, is assumed to consist of components due to suction, temperature, chemical and stress changes. This can be given in an incremental form, without loss of generality, as:

$$d\varepsilon = d\varepsilon_{\sigma} + d\varepsilon_{c_s} + d\varepsilon_s + d\varepsilon_T \qquad (1)$$

where the subscripts σ, c_s, T and *s refer* to net stress, chemical, temperature and suction contributions.

A number of constitutive relationships have been implemented to describe the contributions shown in Eq (1). In particular for the net stress, temperature and suction contributions both elastic and elastoplastic formulations have been employed. To describe the contribution of the chemical solute on the stress-strain behaviour of the soil, as a first approximation, an elastic state surface concept was proposed which describes the contribution of the chemical solute via a elastic relationship based on osmotic potentials.

A numerical solution of the governing differential equations presented above is achieved by a combination of the finite element method for the spatial discretisation and a finite difference time stepping scheme for temporal discretisation. The Galerkin weighted residual method is employed to formulate the finite element discretisation. For the flow and stress/strain equations shape functions are used to define approximation polynomials.

Software

The software package, COMPASS, has been developed to implement the numerical approach detailed above. The package has a modular structure to aid the implementation of suitable code and documentation management systems. It has two main components, namely a pre and post processor and an analysis ‘engine’. Evaluation of integrals is achieved via Gaussian integration. For the elasto-plastic based stress equilibrium equations a stress return algorithm is required.

BRIGHT *(A. Ledesma, CIMNE, ENRESA)*

A porous medium composed by solid grains, water and gas is considered. Thermal, hydraulic and mechanical aspects are taken into account, including coupling between them in all possible directions. As illustrated in Figure 7, the problem is formulated in a multiphase and multispecies approach.

The three phases are:

- Solid phase (*s*): minerals
- Liquid phase (*l*): water + air dissolved
- Gas phase (*g*): mixture of dry air and water vapour

The three species are:

- Solid (-): mineral particles
- Water (*w*): as liquid or evaporated in the gas phase
- Air (*a*): dry air, as gas or dissolved in the liquid phase

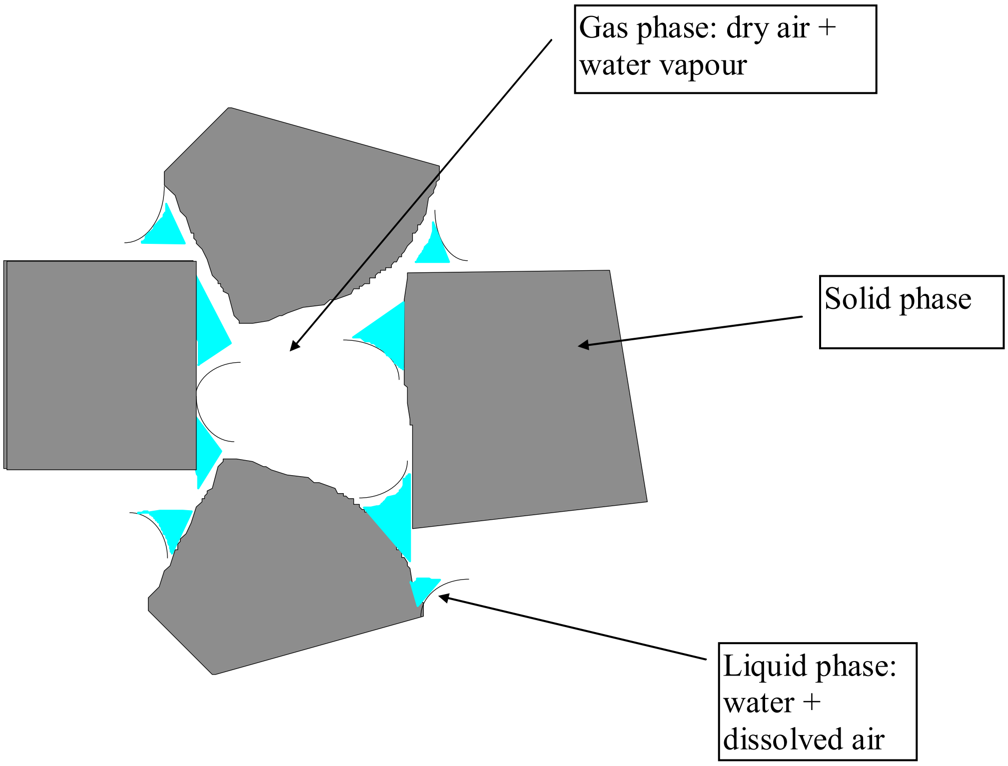


Figure 7. *Schematic representation of an unsaturated porous material.*

The following assumptions are considered in the formulation of the problem:

- Dry air is considered a single species and is the main component of the gaseous phase. Henry's law is used to express equilibrium of dissolved air.
- Thermal equilibrium between phases is assumed. This means that the three phases are at the same temperature
- Vapour concentration is in equilibrium with the liquid phase, the psychrometric law expresses its concentration.
- State variables (also called unknowns) are: solid displacements, u (three spatial directions);liquid pressure, P_l; gas pressure, P_g; and temperature, T.
- Balance of momentum for the medium as a whole is reduced to the equation of stress equilibrium together with a mechanical constitutive model to relate stresses with strains. Strains are defined in terms of displacements.
- Small strains and small strain rates are assumed for solid deformation. Advective terms due to solid displacement are neglected after the formulation is transformed in terms of material derivatives (in fact, material derivatives are approximated as eulerian time derivatives). In this way, volumetric strain is properly considered.

- Balance of momentum for dissolved species and for fluid phases are reduced to constitutive equations (Fick's law and Darcy's law).

- Physical parameters in constitutive laws are function of pressure and temperature. For example: concentration of vapour under planar surface (in psychrometric law), surface tension (in retention curve), dynamic viscosity (in Darcy's law), are strongly dependent on temperature.

The governing equations that CODE-BRIGHT solves are:1) *Mass balance of solid, 2) Mass balance of water, 3) Mass balance of air, 4) Momentum balance for the medium, 5) Internal energy balance for the medium*

Associated with this formulation there is a set of necessary constitutive and equilibrium laws. Table 2 is a summary of the constitutive laws, variables and equilibrium restrictions that have been incorporated in the general formulation. The constitutive equations establish the link between the independent variables (or unknowns) and the dependent variables. There are several categories of dependent variables depending on the complexity with which they are related to the unknowns.

Table 2. Constitutive equations and equilibrium restrictions.

Equation	**Variable Name**
Constitutive equations	
Darcy's law	liquid and gas advective flux
Fick's law	vapour and air non-advective fluxes
Fourier's law	conductive heat flux
Retention curve	Liquid phase degree of saturation
Mechanical constitutive model	Stress tensor
Phase density	liquid density
Gases law	gas density
Equilibrium restrictions	
Henry's law	Air dissolved mass fraction
Psychrometric law	Vapour mass fraction

Basis for formulation of governing equations

The resulting system of partial differential equations is solved numerically dividing the operation into spatial and temporal discretizations. The finite element method is used for the spatial discretization while finite differences are used for the temporal one.

The mechanical stress-strain relationship of the buffer clay is defined by means of an elastoplastic model specially designed for unsaturated soil and known as the "Barcelona Basic Model". The early difference in physical state between the zone with pellets and the blocks of bentonite will be considered by using different parameters but the same model. Rock will be considered elastic in all the analyses.

An attempt to simulate the THMC problem in 1D will be carried out as well, including reactive transport in the problem. The type of processes that can be considered will include complex formation, oxidation/reduction reactions, acid/base reactions, precipitation/dissolu-tion of minerals, cation exchange, sorption and radioactive decay. The total analytical concentrations are adopted as basic transport variables and chemical equilibrium is achieved by minimising Gibbs Free Energy.

BGR *(L. Liedtke, BGR)*

Buffer evolution

Completely coupled thermo/hydraulic/mechanical models considering the non-linear effects caused by i.a. permeation under unsaturated conditions and the elasto/plastic behaviour of the buffer clay are basic to the BGR model. For the buffer one also needs to consider the influence of dessication fractures, swelling and microstructural changes. Major processes in the saturation and subsequent percolation of the buffer are:

- Reduction of the permeable pore space by the expansion of the smectite clay particles and thereby the hydraulic conductivity.
- Changes in effective stress and strain in the saturation phase, which affect the mechanical behaviour of the clay. Here, changes in temperature, water content and stress conditions in both the buffer clay and confining rock play major roles.
- Formation and transport of vapour.
- Osmosis.

The following principles and concepts are basic to the model:

- Effective stress and consolidation concepts (Biot, Terzaghi).
- Mohr-Coulomb failure concept including the influence of internal friction, cohesion, and dilatancy.
- Drucker/Prager's (1952) model of the first invariant of the total stress tensors and the second invariant of stress deviators.
- Roscoe/Schofield/Burland's (1958-1971) Cam-Clay-Model.

Basis for formulation of governing equations

Four unknown field functions are to be determined: gas pressure p_g, water pressure p_W, solid displacements, u, and equilibrium temperature T. In addition to physical changes (stress/strain, drying and wetting) and chemical alteration some of the properties used for modelling, like alteration of the heat conductivity of buffer under saturation, and microstructural changes, have to be taken into consideration.

One can identify impacts in the form of hydromechanical, thermomechanical and hydrothermal effects. For non-isothermal processes in partially saturated porous media it is more convenient to separate dry air and vapour and formulate a mass balance equation for both liquid species, i.e. liquid and liquid vapour.

Concepts for formulations are compositional or phase-related. The first approach consists of balancing the species rather than the phases. The compositional approach is adopted to establish the mass balance equations.

Hydromechanical effects

Water saturation and swelling of the buffer lead to changes on the microstructural level like changes in porosity, hydraulic conductivity and deformation moduli.

Thermomechanical effects

Temperature-dependent dessication changes the stress/strain behaviour of the buffer clay and causes a need for developing thermo-plastic stress/strain material models and extension of the models describing visco-elastic and visco-plastic strain.

Hydrothermal effects

- The most important hydrothermal effects are related to:
- Redistribution of the initial porewater content in the buffer including vapour formation and condensation.
- Changes in viscosity and hydraulic conductivity of water in different temperature regions.
- Influence on porewater pressure and saturation rate by the groundwater pressure in the rock.
- Alteration of the heat conductivity of buffer under saturation.
- Chemical alteration of the porewater and mineral phases (disregarded so far in the model).

Modelling of the Excavation-disturbed Zone with respect to water uptake and hydraulic pressure distribution in the bentonite buffer

A model has been developed for predicting the hydration of the initially unsaturated buffer with respect to the interaction with the surrounding rock. The inflowing water from the rock is distributed over the EDZ, which can be supplied with water from discrete water-bearing fractures that intersect the deposition holes. A basic principle of the model is that the hydraulic behaviour of the EBS system is affected by the saturation of the buffer.

The transient groundwater flow in the system is described by the expression:

$$S_0 \frac{\partial h}{\partial t} + \nabla v = q \qquad (2)$$

where h is the piezometric head, t the time, S_0 the specific storativity, v the average fluid velocity vector, and q the fluid sink/source.

The velocity is given by the three-dimensional, linear Darcy law:

$$v = -K \cdot \nabla h \qquad (3)$$

where K is the hydraulic conductivity tensor, or by the general form of various non-linear laws for fracture or tubular flow:

The finite element method is used for the numerical simulation of transport and time derivatives are evaluated by using different schemes with various order of accuracy. The stability of numerical solutions depends on the reference point in time of difference formulae. In general, a distinction is made between explicit and implicit schemes. A number of approximate schemes with respect to stability and consistency are examined. The Neumann stability criterion states that the intrinsic values of the amplification matrix of the discretised equation must be lower or equal to unity. Important stability criteria are stated in terms of the Courant number *Cr*.

THAMES *(Y. Sugita, JNC)*

General

The mathematical formulation for the model utilizes Biot's theory with the Duhamel-Neuman's form of Hooke's law, and an energy balance equation. The governing equations are derived with fully coupled thermal, hydraulic and mechanical processes. They are derived under the following assumptions:

1. The medium is poro-elastic.
2. Darcy's law is valid for the flow of water through a saturated-unsaturated medium.
3. Heat flow occurs in solid and liquid phases (impact of vapor is not considered).
4. Heat transfer among three phases (solid, liquid and gas) is disregarded.
5. Fourier's law holds for heat flux.
6. Water density varies depending upon temperature and the pressure of water

Rheology

The Terzaghi effective stress principle and Bishop and Blight's extended definitions an equation for saturated and unsaturated media are used:

$$\sigma_{ij} = \sigma'_{ij} + \chi\delta_{ij}\rho_f g\psi \qquad (4)$$

where σ'_{ij} is the effective stress, δ_{ij} is the Kronecker's delta, ρ_f is the unit weight of water, g is the acceleration of gravity and ψ the pressure head. Subscript f means "fluid". The parameter χ is defined as $\chi=1$ (Saturated zone), $\chi=\chi(S_r)$ (Unsaturated zone). χ is a nonlinear function of the degree of saturation (S_r). At present it is assumed that χ is approximately equal to S_r.

The effects of temperature on the stress/strain behaviour of an isotropic linear elastic material follows the constitutive law:

$$\sigma'_{ij} = C_{ijkl}\varepsilon_{kl} - \beta\delta_{ij}(T - T_o) \quad (5)$$

where $\beta = (3\lambda+2\mu)\alpha_T$. C_{ijkl} is the elastic matrix, ε_{kl} the strain tensor, T the temperature, λ and μ Lamé's constants, and α_T the thermal expansivity coefficient. Subscript o means that the parameter is in a reference state.

Moisture transport

The equation of porewater motion is expressed by Darcy's law. The physico/chemical state of the gaseous phase in soil is too complicated to be modeled and in the present case pores in the buffer clay are assumed to be filled with only a liquid phase. This means that the ground water does not change in phase from liquid to gas or vise versa and that the thermal conductivity of the gaseous phase is disregarded. Since the heat conductivity of the gaseous phase is smaller than that of the liquid and solid phases, the heat conductivity of the composite material is not affected much by the volume of the gaseous phase.

Basis for formulation of governing equations

The behavior of the buffer material is influenced by the interdependence of thermal, hydraulic and mechanical phenomena. To treat the water/vapor movement and heat induced water movement, the continuity equation used in the extended THAMES code contains terms representing the isothermal water diffusivity D_θ, the volumetric water content θ, the water potential head ψ, and is the intrinsic permeability K. This equation means that the water flow in the unsaturated zone is expressed by the diffusion term and in the saturated zone by the Darcy's law.

The stress/strain relationship at equilibrium takes the swelling behaviour into account and considers the elastic matrix, the density of the medium and the body force. The effective stress in the unsaturated zone and in the saturated zone are functions of the thermal expansion. The swelling pressure is assumed to be a function of the water potential head.

ABAQUS *(L. Börgesson, Clay Technology AB, Lund, Sweden (SKB)*

General

The finite element on ABAQUS model has been extended to include special material models for rock and soil and an ability to describe moisture transport associated with stress and strain on various scales. The hydro-mechanical model consists of a porous medium and wetting fluid and is based on equilibrium, constitutive equations, energy balance and mass conservation using the effective stress theory.

The simplified equation used in ABAQUS for the effective stress is:

$$\bar{\sigma}^* = \sigma + \chi\, u_w \mathbf{I}. \qquad (6)$$

where σ is the total stress, u_w is the porewater pressure, χ is a function of the degree of saturation (usual assumption $\chi = S_r$), and **I** the unitary matrix.

Moisture transport

Vapour flow is modelled as a diffusion process driven by a temperature gradient. Flow of liquid water is expressed in terms of Darcy's law corrected with respect the degree of water saturation.

Coupling of thermal and hydro-mechanical solutions

In ABAQUS the coupled problem is solved through a ”staggered solution technique” as shown in Figure 8.

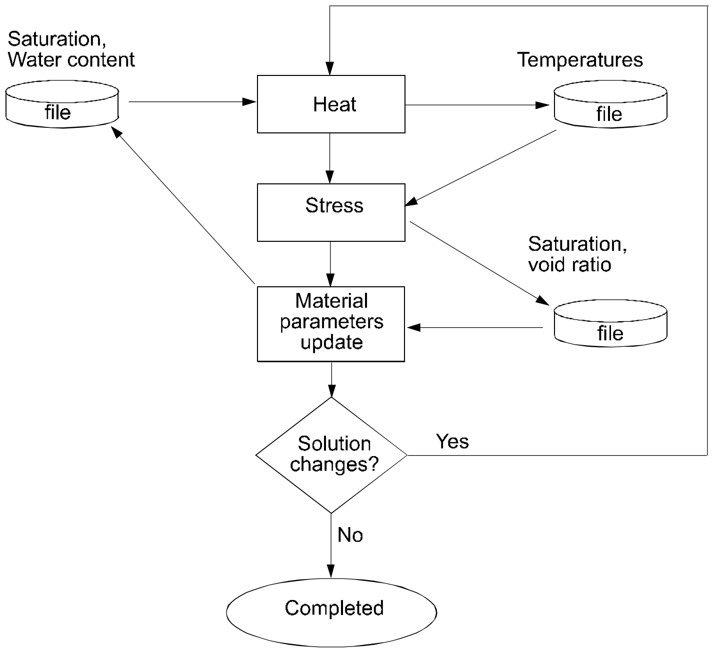


Figure 8. *In ABAQUS, heat transfer calculations and hydro-mechanical calculations are decoupled. By using the iteration procedure schematically shown above, the effects of a fully coupled THM model are achieved.*

Basis for formulation of governing equations

Heat transport

Thermal flux by conduction is modelled using conventional theory with thermal conductivity and specific heat as variables.

Moisture transport

The water flux in the liquid phase is modelled by Darcy's law with the water pressure difference as driving force in the same way as for water saturated clay. The magnitude of the hydraulic conductivity K_p of partly saturated clay is a function of the void ratio, the degree of saturation and the temperature. K_p is assumed to be a function of the hydraulic conductivity K of saturated clay and the degree of saturation S_r.

Water vapour flow is modelled as a diffusion processes driven by the temperature gradient and the water vapour pressure gradient (under isothermal conditions).

Hydraulic coupling between the pore water and the pore gas

The pore pressure u_w of the unsaturated buffer material is always negative and expressed as a function of the degree of saturation S_r independently of the void ratio. ABAQUS also allows for hysteresis effects, which means that two separate curves may be given (drying and wetting curves).

Mechanical behaviour of the particle skeleton

The mechanical behaviour has been modelled with a non-linear Porous Elastic Model and Drucker-Prager Plasticity model. The effective stress theory as defined by Bishop is applied and adapted to unsaturated conditions. The shortcoming of the effective stress theory is compensated for by a correction called "moisture swelling" that is a function of the degree of saturation.

Thermal expansion

The volume change caused by the thermal expansion of water and particles is modelled but only expansion of the separate phases is taken into account. The possible change in volume of the particle structure assembly by thermal expansion (not caused by expansion of the separate phases) is not modelled. However, a thermal expansion in water volume will change the degree of saturation, which in turn will change the volume of the structure.

Chemical model *(A.Lukkonen, POSIVA)*

The modelling task is divided into two parts. Analysed water samples from the near-field rock from March 1998 to spring 2002 around the Sections 1 and 2 are used for inverse geochemical calculations in order to deduce the mixing evolution of various local reference water types and the proper reaction amounts for the appropriate reacting phases. Inverse modelling is done by use of the PHREEQC-2 software and supported with C, S-isotope fractionation calculations with NETPATH if applicable.

The target of predictive forward modelling is from the spring 2002 onwards. The knowledge extracted from the inverse calculations and the data collected during March 1998 – spring 2002 are used to calibrate the predictive modelling in the studied sampling points. Although, there will be material for model calibration, the predictions shall be essentially "blind predictions" in nature. The effects of backfill and heat up to the near-field groundwater must be estimated based on a priori theoretical knowledge. For example, Huertas et al have specified certain properties of the VOLCLAY bentonite. Similarly, they have recently reported the effects of heating of a repository in the FEBEX project.

The modelling software will be PHREEQC-2. The predictions can be made either as batch mixing/reaction studies or as 1D mixing/reaction path studies. In the case of batch mixing/reaction studies the predictions concentrate on individual near-field sampling points. The evolution of mixing fractions and reactions are predicted in these points without considering the hydraulic flow field quantitatively. In the case of 1D reaction/mixing path studies the predictions concentrate to the series of near-field sampling points along a hydraulic flow field. The studies then attempt to predict how the changes in mixing fractions and reactions move in the flow field as a function of time. The thermodynamical databases available for the forward PHREEQC-2 studies are e.g. WATEQ4F.DAT EQ3/6 compatible LLNL.DAT (based on "thermo.com.V8.R6.230" by Jim Johnson, LLNL) and NAGPSI_1.DAT (Pearson & Waber).

So far focus has been on the initial geochemical conditions establishing a solid basis for the further studies of the operational repository. Moreover, the blind prediction exercise of the effects of the operational repository tests make up several cornerstones of the predictive modelling. The validity of the model formulation, the possible deficiencies in the thermodynamic databases, and the capabilities of modelling tools are all included in the test.

2.3 Application of theoretical models for predicting the EBS evolution

All parts have been using their respective models for predicting the EBS evolution and the present chapter gives examples of the results.

UWC:

Generic repository – temperature and porewater pressure

This describes the period after deposition hole excavation and prior to the emplacement of the canisters and buffer, when the hydraulic regime of the rock mass will develop. Processes to be addressed include the flow of moisture from the rock mass into the tunnel and deposition holes. This transfer of moisture from the rock may occur in both the liquid and vapour phase. Both of these processes can be addressed. The effect of desaturation on the moisture retention capacity and hydraulic conductivity of the rock mass can be considered. Also, the influence of the EDZ can be taken into account. Geometry and boundary conditions required include: geometry of deposition holes and tunnel; duration of excavation stage; location and extent of fractures and EDZ; initial pore water pressure in rock; far field hydrostatic pore water pressure in rock; relative humidity and temperature of the tunnel and borehole.

The descriptive example investigated here involves the placement of a full-size heater in a 5 m deep borehole with a bentonitic buffer material (Figures 9 and 10). The example has been divided into three distinct phases; the construction of the facility, a 'dwell' period to allow stabilisation of pore water pressures between the buffer, and the rock, and a heating period.

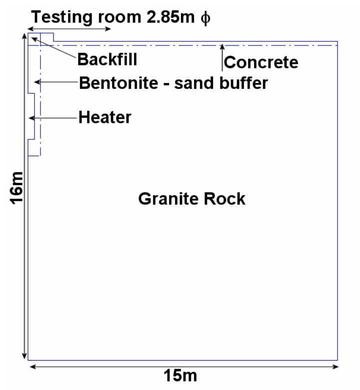


Figure 9. *Axisymmetric domain of basic rock/buffer/backfill/heater system .*

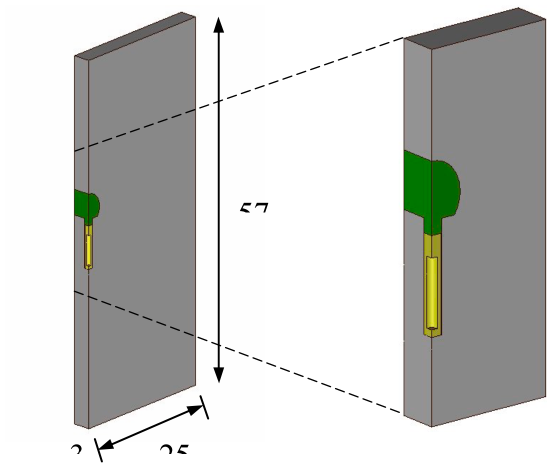


Figure 10. *Tunnel and rock section used for the thermal analysis and enlarged view of cross-section.*

The geometry of the model for FEM calculations is shown in Figure 11.

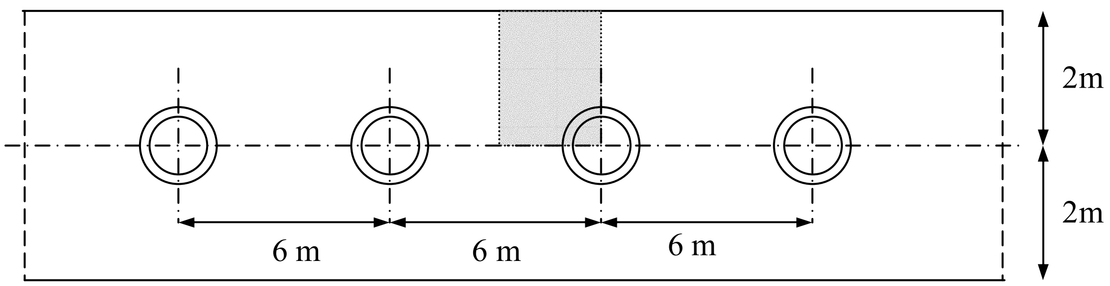


Figure 11. *Schematic plan view of tunnel floor used for the generalised 3D model (not to scale).*

The calculations were based on the following data:

- The initial temperature throughout the domain was set at 287 K (14°C).
- The heat generation of the electric power 1800 W was taken to correspond to a flux of 102 W/m^2
- Material properties as given by SKB

Temperature plots (Figures 12 and 13) at 10 years across a vertical cross-section perpendicular to the tunnel axis shows a maximum heater temperature of 376 K (103°C).

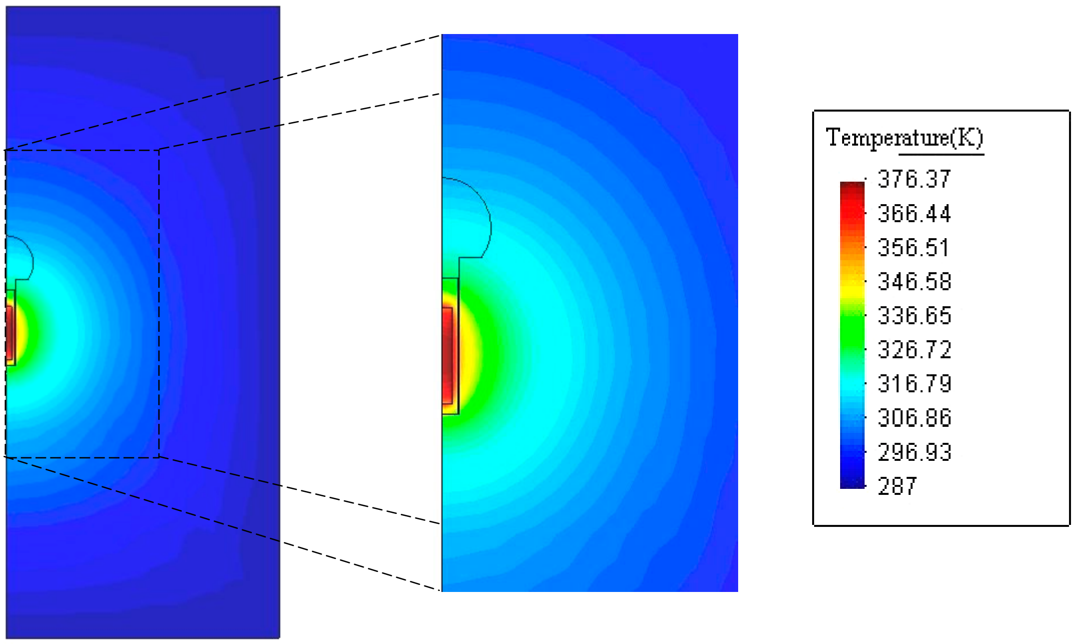


Figure 12. *Temperature plot after 10 years.*

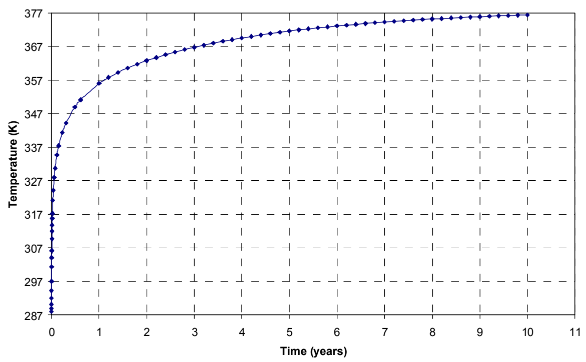


Figure 12. *Temperature on the canister surface.*

The numerical modelling followed the phases of construction, with the influence from the construction of the underground caverns considered first. Following placement of the buffer a dwell period of 170 days was modelled. Results show that during the dwell period desaturation will occur within the rock for a distance of approximately 1.5 m from the centre of the heater. Finally, the heating stage was addressed via a coupled temperature and mass analysis.

3D hydraulic analysis

The work has also comprised a 3D hydraulic analysis of a generalised tunnel section (Figure 14) for simulating the inflow into each of the boreholes and for predicting the initial conditions of the heating stage of the experiment.

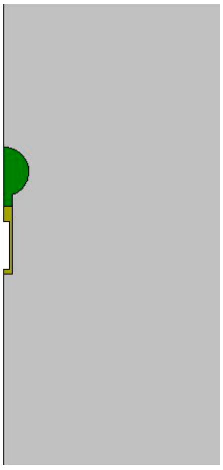


Figure 14. *2D axisymmetric geometry.*

The boundary conditions along the edges of the far-field rock were restrained and the porewater pressure was set to a hydrostatic value. This boundary was located at a suitable distance so that the applied condition did not influence the results. An adiabatic boundary was prescribed on the three surfaces of the section containing the tunnel so as to represent the axes of symmetry in the system. Hence, effectively an infinite line of deposition holes was modelled. The surface of the tunnel and boreholes where set at zero porewater pressure.

Figure 15 shows a pore water pressure plot across a vertical cross-section perpendicular to the tunnel axis at steady state conditions.

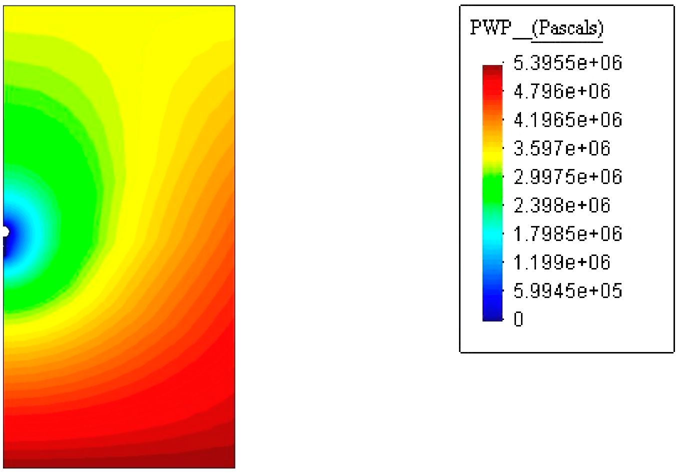


Figure 15. *Pore water pressure plot for a hydraulic conductivity of E-12 m/s.*

Table 3 shows the predicted inflow into the boreholes for various assumed hydraulic conductivities. The inflow naturally increases with increasing rock permeability with values varying between 0.00662 and 0.137 l/min. The actual maximum inflow of 0.079 l/min would mean that the average rock conductivity is about E-10 m/s for a rock volume of a few hundred cubic meters, including the effect of discrete fractures.

Table 3. Calculated borehole inflow.

Rock hydraulic conductivity m/s	Borehole inflow (l/min)
E-12	0.00011
E-11	0.001
E-9	0.137
E-12 and Fracture E-8	0.0018

Figure 16 shows a typical representation of a pore water pressure plot at the heater – buffer interface at a mid-heater height. Figure 17 shows the development of temperature at the same point. It can be seen that initial drying is progressively overwhelmed by inflow from the host rock leading to eventual saturation. A peak in temperature can be seen when the buffer is at its driest. This demonstrates the effect of coupling between the hydraulic field and the temperature field.

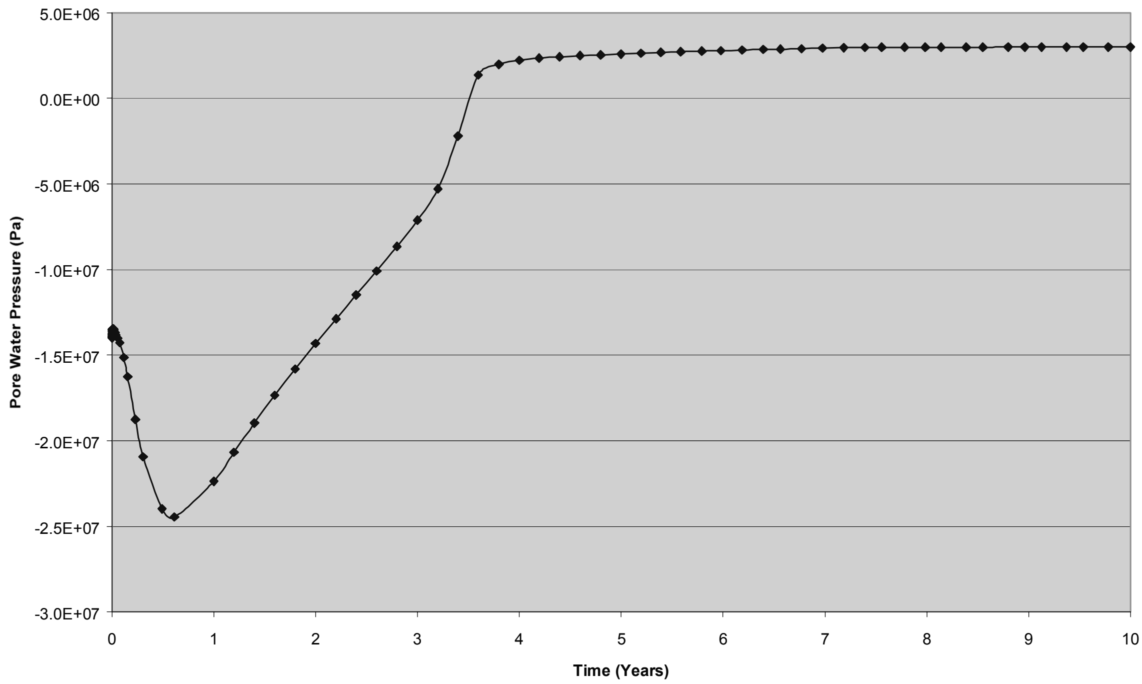


Figure 16. *Pore water pressure plot at the surface heater – buffer interface at mid-heater height.*

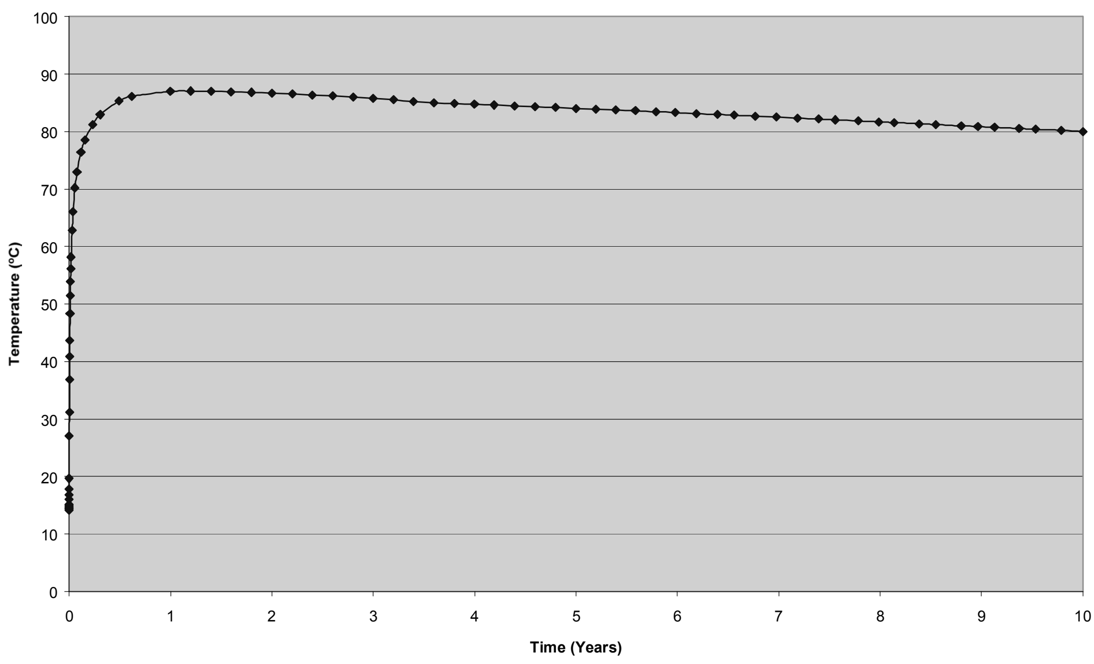


Figure 17. *Temperature plot at the heater/buffer interface at mid-height of the heater.*

CIMNE:

General

TH and THM analyses have been made including variation of the buffer parameters for the pellet filling. So far, a 2D case with two deposition holes has been performed considered for the TH work, while a 1D case has been analysed with respect to THM performance. The various cases refer to geometrical definitions shown in Figure 18.

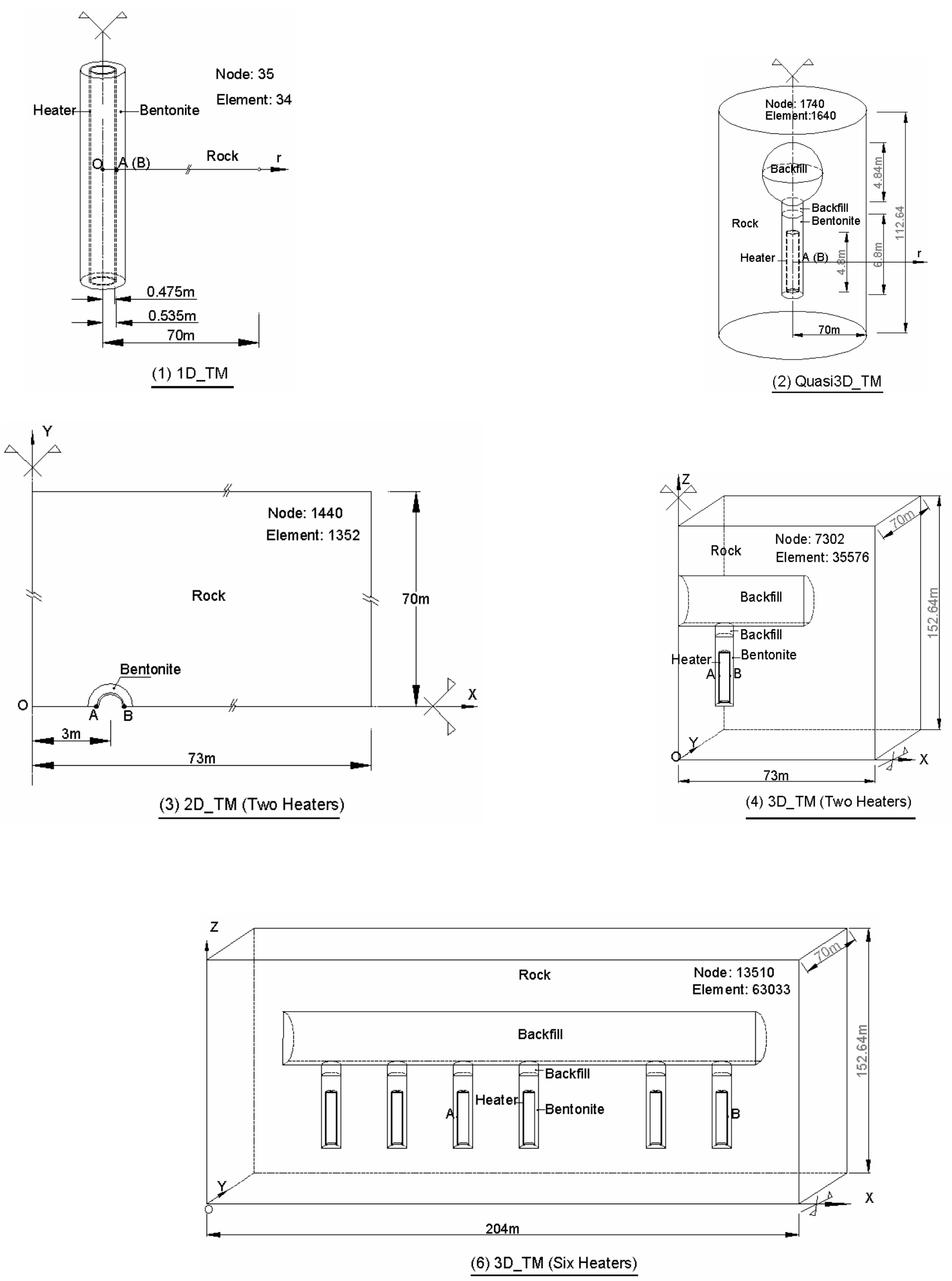


Figure 18. *Geometries considered in the T and TM analyses.*

For T and TM rock analyses the following data were assumed:

- Initial temperature 12 ºC, boundaries located around 70 m away from the holes.
- A constant power 1800 W/heater.
- No gravity or initial stresses exist.

The major results of the T and TM rock calculations can be summarized as follows:

- The axisymmetric case provides reasonable results.
- TM behaviour is mainly controlled by the thermal expansion.
- TM-stress and strain yield maximum values within one year already.

Figure 19 shows the rock temperature evolution.

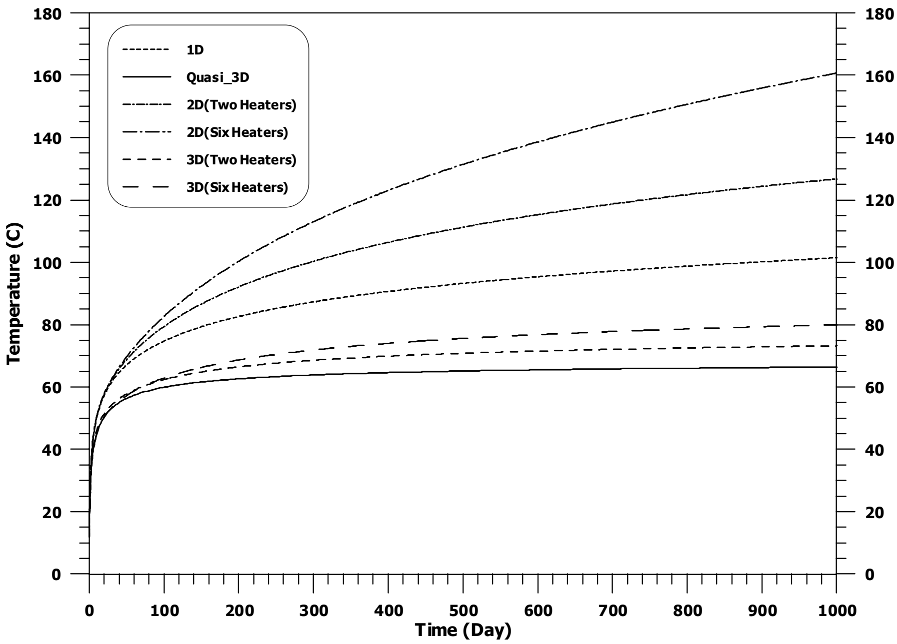


Figure 19. *Evolution of temperature in the hottest part of the rock for different cases.*

TH modelling in 2D

The major results are shown in Figures 20 and 21. They are interpreted in the following way:

- The buffer becomes practically saturated in about 5 months.
- The temperature rises significantly even after 3 years and is higher than 100°C at mid-height canisters.
- The initial drying of the buffer near the canisters is obvious and appears to be in agreement with earlier field experiments [5]

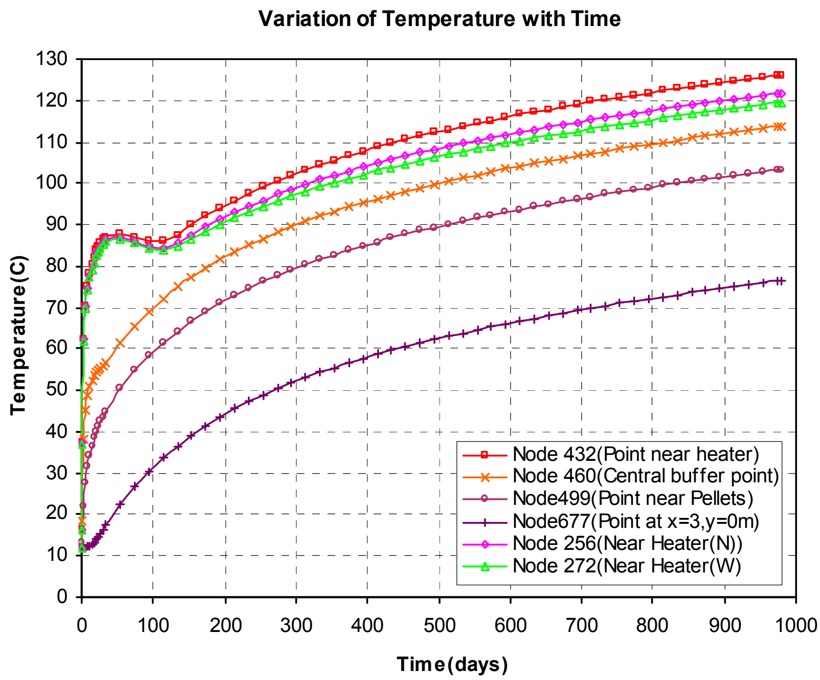


Figure 20. *Temperature vs. time for different points. The temperature at the canister surface passes 125°C after about 3 years.*

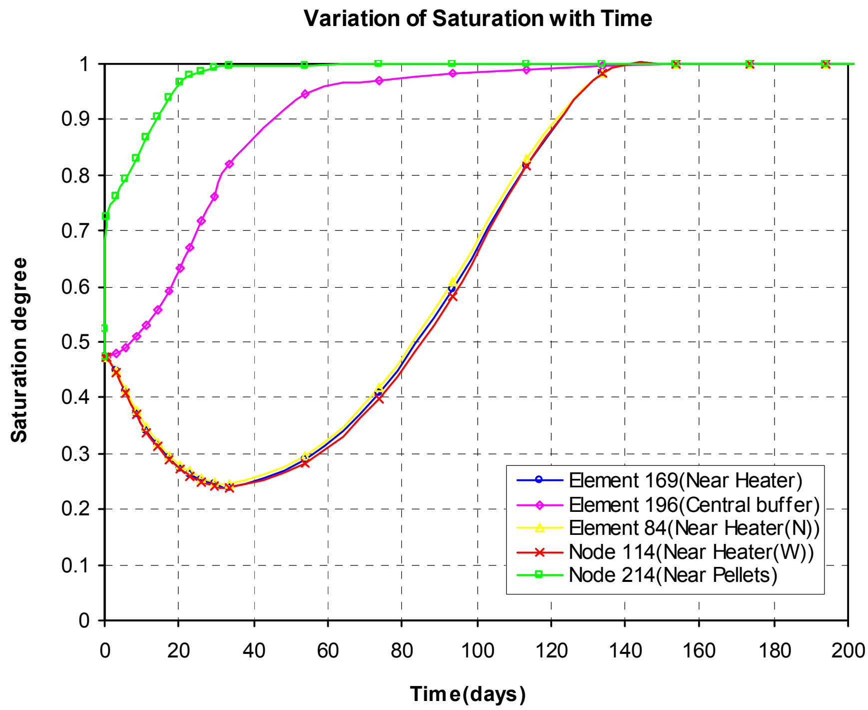


Figure 21. *Degree of saturation vs. time for different points. The degree of saturation of the pellet filling is complete after about 1 month while it takes about half a year to reach this state for the buffer near the canister.*

Results from THM modelling in 1D

The case considered represents an element consisting of pellet filling and buffer clay that extends all the way to the canister. The major results are shown in Figures 22, 23 and 24. They are interpreted in the following way:

- The buffer becomes practically saturated in about 5 months.
- The temperature rises even after 3 years and is higher than 100^{o}C at mid-height canisters. A first maximum is reached after about 2 months; it is related to the performance of the pellet filling.
- Consolidation of the pellet filling requires at least tens of years, indicating that the stress/strain behaviour of the buffer components is different from the real ones (The filling is completely consolidated in a few months).

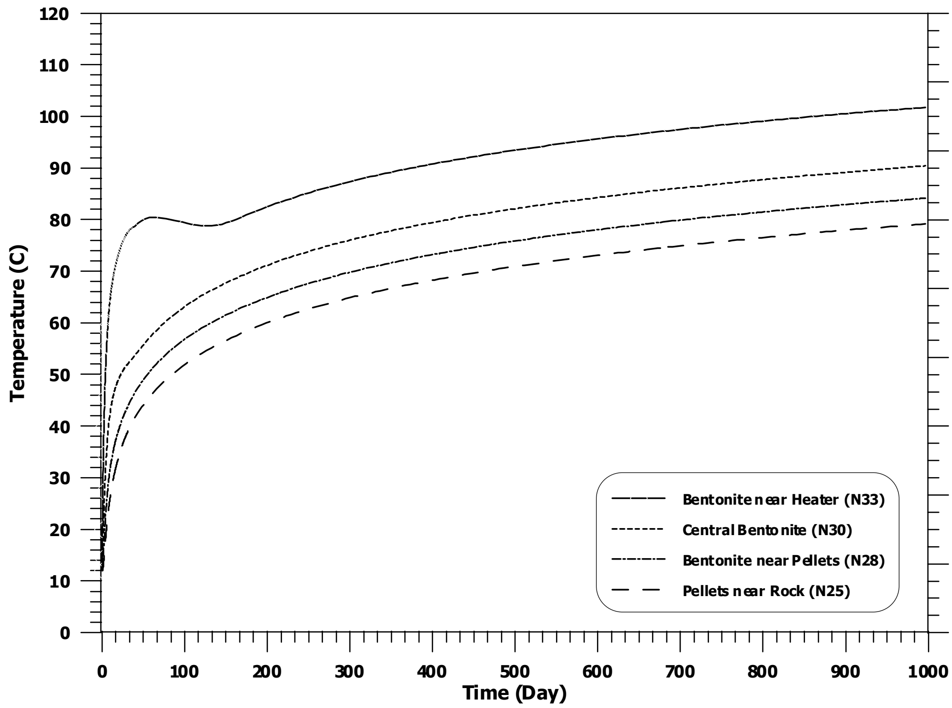


Figure 22. *Change in temperature with time (1800W/Heater).*

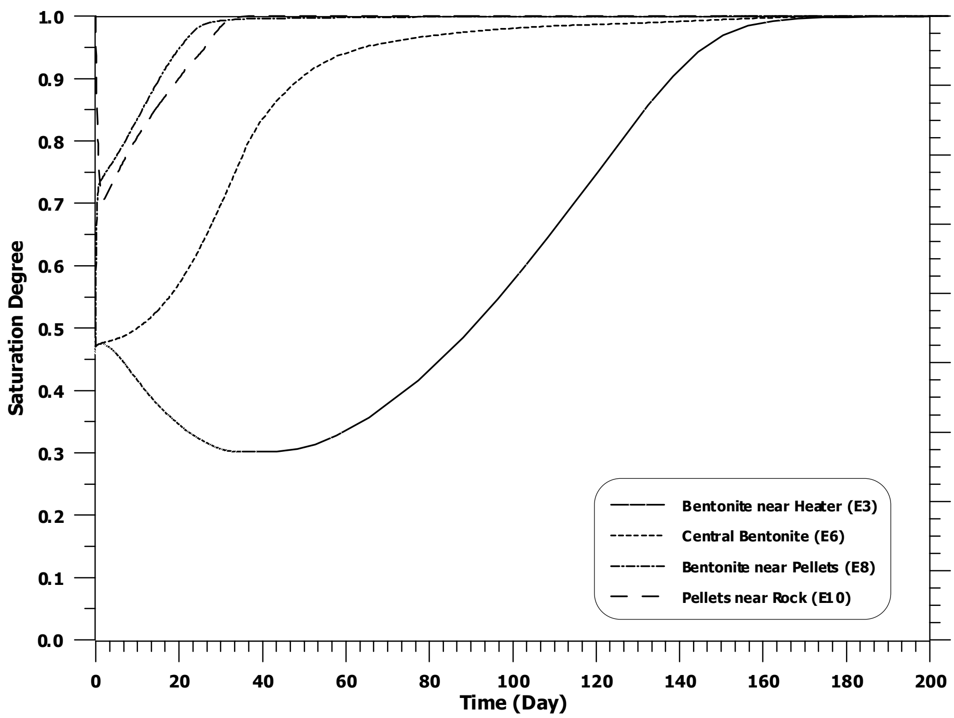


Figure 23. *Change in saturation degree with time (1800W/Heater).*

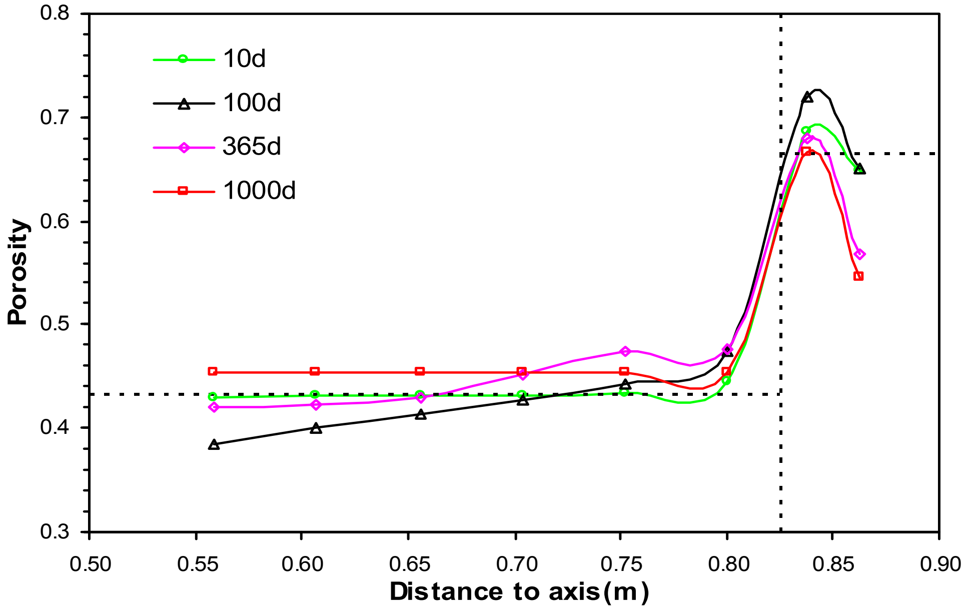
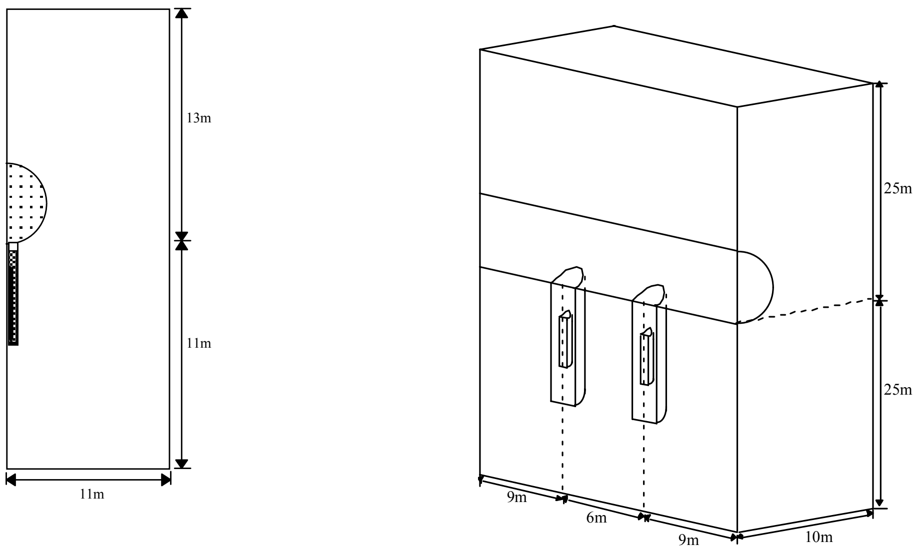


Figure 24. *Bentonite and pellets porosity distribution (1800W/Heater). The porosity of the buffer blocks is changed considerably in 3 years while that of the pellet filling is changed rather little in this period.*

JNC:

THM analyses in 2D (axial symmetry) and 3D

The case considered for analysis is shown in Figure 25. Figure 26 shows a model used for a pilot study.



Two-dimensional

Three-dimensional

Figure 25. *Analysis model.*

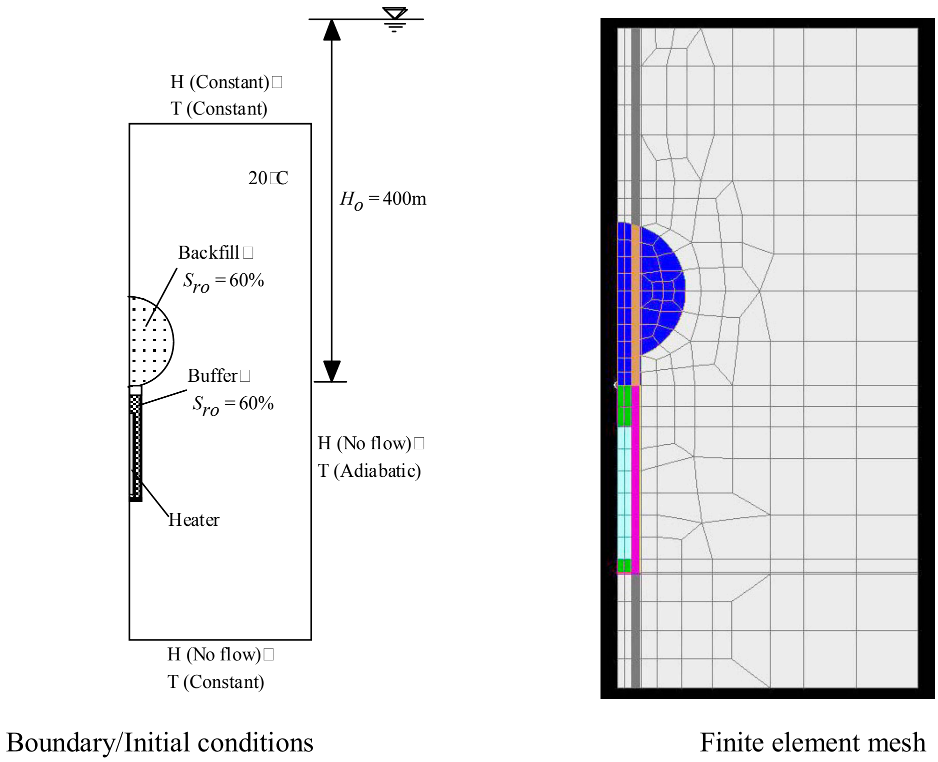


Figure 26. *Model for pre-analysis.*

The conditions and data used for calculations are:

- The boundary conditions were adiabatic and constant water pressure condition in the top, and adiabatic with no flux at the side and bottom.
- The temperature of the surface of the heater was fixed at 100°C.
- The initial conditions were: The total pressure head was 400 m throughout the model. The initial degree of saturation of the buffer and the backfill was 60 % and the temperature 20°C.
- The intrinsic permeability K (m^2) is as a function of void ratio (K=1.81E-20(e)$^{4.3}$.).
- Swelling pressure data from SKB tests, evaluated by THAMES.

The major results from preliminary analyses can be summarized as follows:

- Temperature increases beyond 10 years.
- Temperature at rock/buffer rises to more than 60°C.
- Water content changes as in Figure 27.
- The code THAMES is being improved.

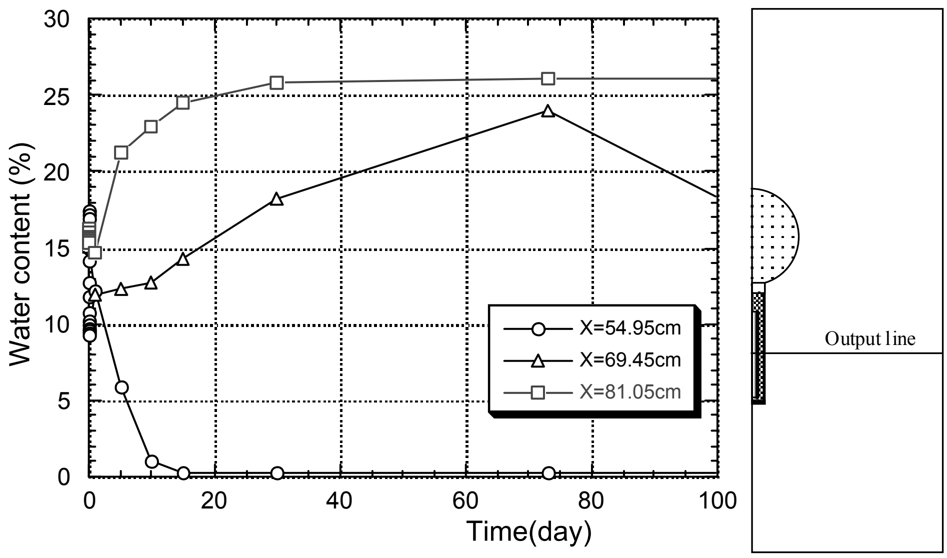


Figure 27. *Water content as a function of time (0-100 days).*

The predicted change in water content of the buffer implies complete drying at the buffer/canister interface in about 3 weeks and complete saturation at the buffer/rock interface in the same period of time. At the midst of the buffer the water content is increased to near saturation in somewhat less than 3 months. In its present form the code is concluded to indicate too rapid water transport in the buffer.

BGR:

THM analysis of rock interacting with buffer

The rock structure and associated groundwater flow paths form the basis for THM calculations that have been performed. The structure is characterized by 18 discrete water-bearing discontinuities called fracture zones here (Figure 28).

The basic assumptions for the calculations which refer to a hole with a steep major fracture have been:

- Water uptake by buffer is from the tunnel, hole-intersecting fractures, and the EDZ. The rock matrix is impermeable.
- The non-steady state hydraulic behaviour of the system is controlled by the saturation of the bentonite.
- Initial and final water contents are 15 % and 25 %, respectively.
- Hydraulic conductivity of saturated bentonite K=E-13 m/s.
- The diagonally located fracture has a hydraulic opening of 200 µm.
- Physical data are those provided by SKB.

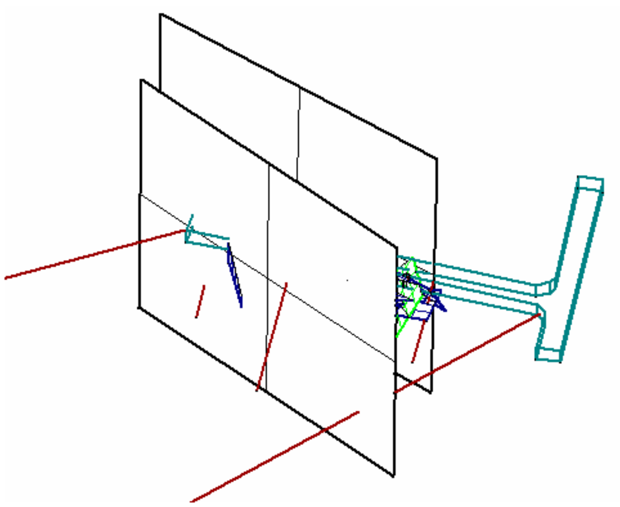


Figure 28. *Prototype repository test field with some hydraulically relevant fracture zones.*

The components are shown in the FEM mesh picture in Figure 29. The system comprises 2D planar fracture elements, spatially curved 2D elements which represent the EDZ and 3D spatial elements. The 3D elements are used to simulate the hydraulic behaviour of the bentonite. The rock mass was taken to be impermeable.

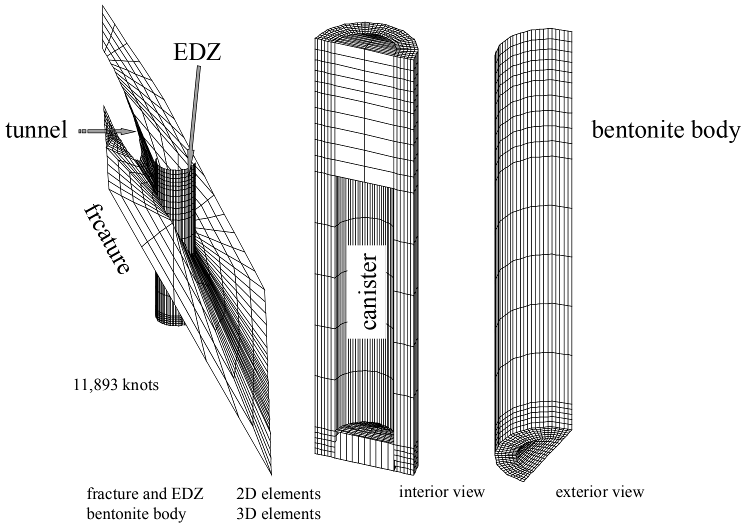


Figure 29. *Finite Element mesh of deposition hole.*

The hydraulic boundary conditions were taken as follows:

- The water pressure in the tunnel and in the fracture remains constant at 1 MPa.
- The specific storativities are: Bentonite S_0 = 0.1, Fracture S_0 = 0.0, EDZ S_0 = 0.0.
- The EDZ data are: 1) thickness (w) 3 mm with *K*= E-9 m/s, 2) thickness 10 mm with *K*=E-10 m/s, 3) thickness 30 mm with *K*=E-11 m/s.

Saturation of buffer

Based on the conductivity data the saturation of the buffer clay and the pressure distribution in the deposition hole were calculated by performing 3D calculation using the two-phase-flow program "ROCKFLOW 3". The results indicated saturation of the bentonite buffer after 5 - 30 years.

The results of the hydraulic calculations were used as input parameters for the mechanical calculations using the ADINA finite element program from MIT. The build-up of stress over time due to bentonite swelling was found to be similar to the results of the two-phase-flow calculations. Two cases were investigated: When expansion was restricted the vertical principal stress above the deposition canister rose to 10 MPa, and in the unrestricted case it was 0 MPa. The three principal stresses varied insignificantly in the former case. In the latter the minor principal stress rose insignificantly, and dropped again after five years to 5.5 MPa. Stress changes and displacements as a result of temperature changes are insignificant in the buffer because of the low value of the coefficient of thermal expansion.

Assuming the water pressure in the fracture and the tunnel to remain at 1 MPa, and applying different storage coefficients and assuming the EDZ to have a thickness of 3-30 mm and a conductivity of E-11 to E-9 m/s the pressures in the system were calculated as a function of time. The time for build-up of relevant piezometric pressures was found to be very long, which can be ascribed to the assumption that the rock matrix is impermeable. Further analyses are being made with different assumptions as to the hydraulic properties of the rock. An early result in the reporting period is shown in Figure 30.

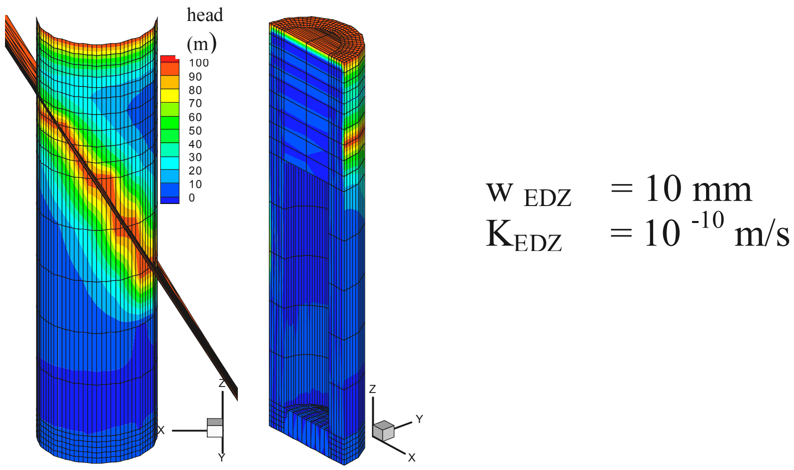


Figure 30. *Distribution of hydraulic head (m) in an EDZ w = 10 mm after a few years. The pressure is high only in the uppermost part of the bentonite and in the part of the EDZ that is adjacent to that fracture.*

The purpose of the study was to make a first estimate of the importance of the EDZ with respect to its function as water source for wetting the unsaturated bentonite. The present assessment of the water-bearing capacity of the EDZ considering the detailed rock structure and measured hydraulic conductivity is that although the most shallow, 10 mm thick part is at least 100 times more permeable than undisturbed rock samples, the modelling indicated that it is not particularly effective in supplying the buffer with water.

Hydration of buffer by diffusive uptake of water with simultaneous inflow by water under pressure, latter attempts

Figure 31 illustrates a case modelled by Lutz Liedtke, BGR, as part of SKB's Prototype Repository Project activities. It represents the conditions in a segment of a KBS-3 tunnel and deposition hole intersected by two water-bearing fractures that interact with a major fracture zone through a system of fractures. For the theoretical case with a hydraulic pressure of 1 MPa, saturation of the buffer to 85 % requires 8 years. If the pressure in the EDZ is very low, saturation will not have gone up to 80 % even after 30 years.

The importance of the EDZ for providing the buffer clay with water for saturation is hence obvious. The pressure conditions are particularly important in this respect and a tentative conclusion is that there are great advantages in backfilling a repository of this type as soon as possible after deployment of the canisters for early saturation of the buffer.

The work performed has included prediction of the rate of changes of the porewater pressure in the rock, buffer and backfill under different hydraulic boundary conditions related to the rock structure.

The boring-induced EDZ extends only to a depth of a few tens of millimeters but yet appears to have an impact on the distribution of water taken up by the buffer as concluded from the Stripa Project [5]. Still, the major water-supplying components in the rock are discrete water-bearing fractures that intersect the deposition holes or the EDZ including stress-induced fractures and fissures.

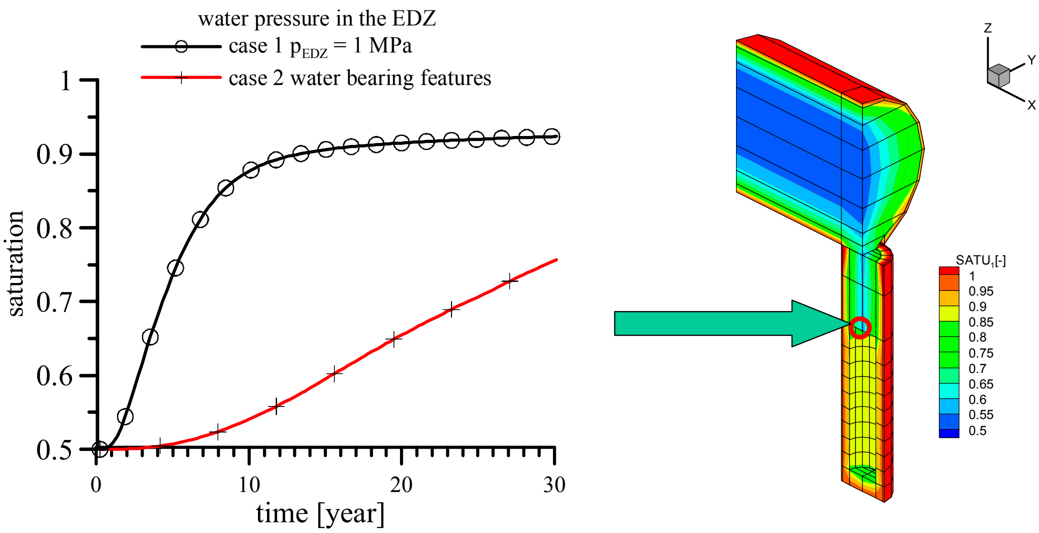


Figure 31. *Water saturation versus time for the case of continuosly pressurized EDZ in KBS-3 deposition hole by 1 MPa, and the case with virtually no pressure and water uptake through 2 water-bear fractures (Calculation by Lutz Liedtke, BGR).*

Clay Technology:

HM-modelling of the buffer hydraulically interacting with rock

Rock with no fractures but with an EDZ with a hydraulic conductivity of E-10 m/s within 10 mm from the walls of a deposition hole, and rock with two subhorizontal fractures intersecting the hole, have been considered in early calculations using the ABAQUS code. The outcome of the calculation of porewater pressure is illustrated in Figure 32. They show that the negative water pressure in the rock after 4 years with and without fractures is still very substantial, particularly in the fracture-free case. In practice, it is believed that the there is a sufficiently high number of water-bearing features – finer fractures and fissures – to even out the underpressure early in the buffer saturation phase. One therefore concludes that it still remains to work out a relevant rock structure for applying this and other codes in THM calculations.

THM-modelling of the buffer saturation

Earlier application of the ABAQUS code shows that it may take between a couple of years and more than 20 years to reach 95 % degree of saturation depending on the ability of the rock to give off water to the buffer, the external water pressure, and the hydraulic performance of the EDZ.

Figure 33 (upper part) shows the predicted degree of water saturation as a function of the radial distance from the centre of the canister top after 0.5 years (/2), 1.0 year (/3), 2.0 years (/4), 4.0 years (/5), 8.0 years (/6), 16.0 years (/7), and 32.0 years (/8) years assuming rock with no fractures.

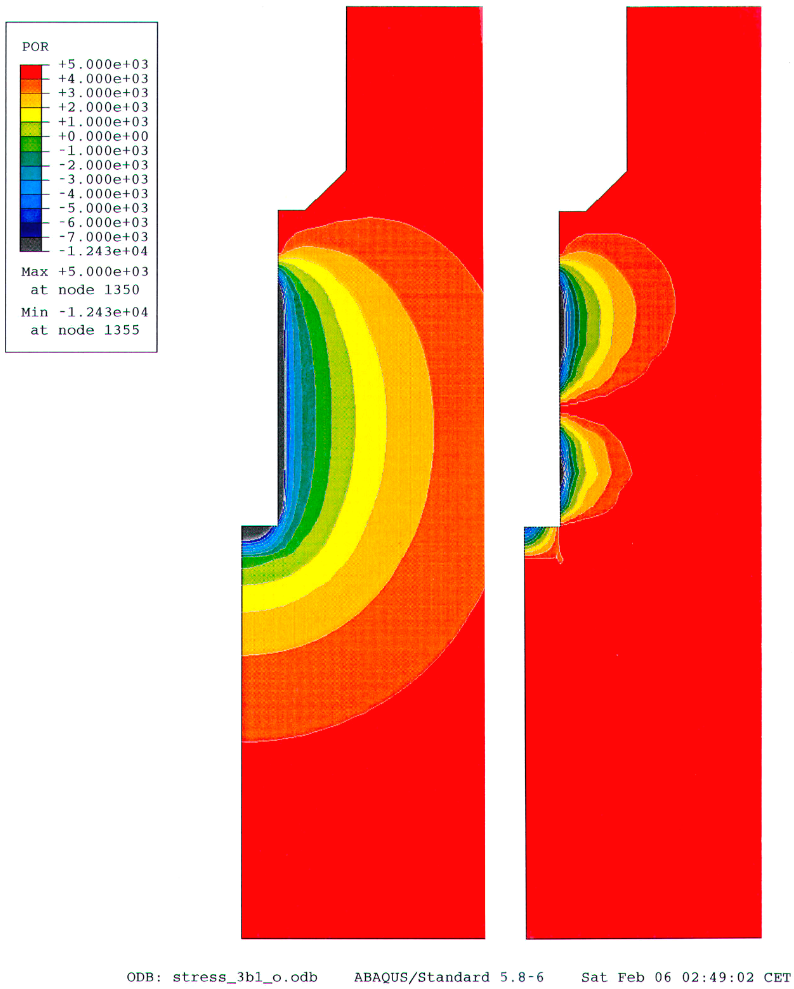


Figure 32. *Pore water pressure (kPa) in the rock after 4 years without fracture (left) and with fracture. The suction in the rock is tremendous.*

HM-modelling of rock, buffer and canister – displacement of canister

The expanding buffer displaces the canister and backfill. Figure 33 (lower part) shows the predicted displacement (in meters) of the canister (green) and of the boundary between the buffer and backfill (red) as a function of time (s). The upheaval of the interface between buffer and backfill is predicted to be on the order of 7 cm after about one year and stay so for any period of time, and that the canister will move up by a couple of centimeters in half a year and then sink back.

The predicted upward expansion causing displacement of the backfill seems to be in agreement with measurements in the Stripa BMT field experiments where the movement was found to be 7 cm in about 4 years. The geometries and material properties were somewhat different but the overall conclusion is that the model appears to be applicable.

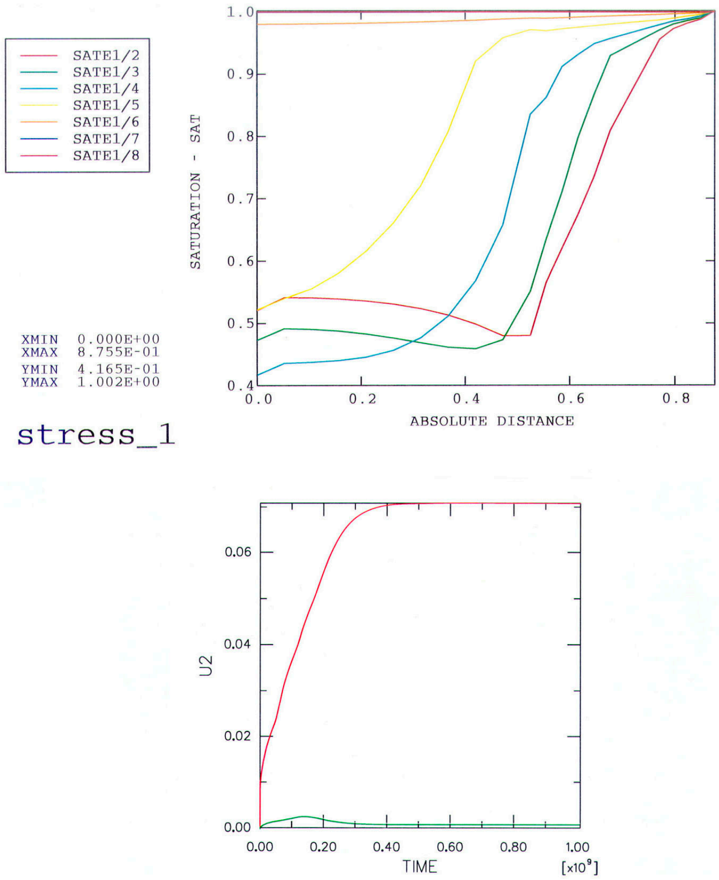


Figure 33. *Upper diagram: Degree of saturation as a function of the radial distance from the centre of the canister top after 0.5 years (/2), 1.0 year (/3), 2.0 years (/4), 4.0 years (/5), 8.0 years (/6), 16.0 years (/7), and 32.0 years (/8) years. Lower diagram: Displacement (m) of the canister (green) and the centre of the boundary between the buffer and backfill (red) as a function of time (s). Calculations made by Börgesson and Hernelind.*

VTT/TVO:

C modelling of buffer, backfill and groundwater

The VTT-POSIVA predictive modelling relies on laboratory studies of VOLCLAY - bentonite and porewater compositions. The modelling attempts to take into account the following geochemical aspects: ion-exchange, surface complexation and dissolution-precipitation reactions. At present the modelling method and the boundary conditions have been conceptualised. The first predictions have been made but the calibration of the calculation model with respect to laboratory studies is not yet finished.

3 Comments

The following general conclusions can be drawn from the application of the THMCB models:

- The redistribution of porewater in the early water saturation phase of the buffer is similar for all the models.
- The temperature evolution is similar for all the models but the ultimate temperature and the time to reach it varies considerably.
- The rate of water saturation in later phases is different for different models. The discrepancies are due to different assumptions with respect to the performance of the EDZ.
- C- and B modellings have not been reported yet.

4 References

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