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Äspö Hard Rock Laboratory

Prototype Repository

Selection of THMCB models

Roland Pusch, ed.

Geodevelopment AB

August 2001

Svensk Kärnbränslehantering AB
Swedish Nuclear Fuel
and Waste Management Co
Box 5864
SE-102 40 Stockholm Sweden
Tel +46 8 459 84 00
Fax +46 8 661 57 19

Äspö Hard Rock
Laboratory

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Roland Pusch (ed.)
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1. ABSTRACT

The evolution of the KBS3 buffer and backfill is going to be modelled with respect to temperature (T), water migration (H), stress and strain (M), as well as to chemistry (C) and biology (B). Five THM- models have been proposed to be used by the individual Parts engaged in the study and some of them also include possibilities to add chemical processes in the buffer evolution. One model deals solely with water chemistry. The present document summarizes the major features of the models without assessing them. The basis for selection and development of these numerical tools for predicting and evaluating the processes in these engineered barriers is a simplified conceptual model.

2. SAMMANFATTNING

Mognaden av bufferten och återfyllningen i KBS-3, speciellt för fallet Protype Repository Project, kommer att modelleras med avseende på temperatur (T), vattenmigration (H), speänningar och deformationer (M), såväl som kemi (C) and biologi (B). Som grund för val av lämpliga parametervärden och relevanta scenarios har en konceptuell modell formulerats. Fem THM-modeller har beskrivits av Parterna som ingår i studien och några av dem ger också möjlighet till att behandla kemiska processer i buffertutbildningen. En av modellerna rör uteslutande vattenkemin.

En särskild svårighet är att bedöma den hydrauliska funktionen hos omgivande berg, som ger randvillkoren. För kalibrering av modellerna kommer resultaten från "Återtagsförsöket" och det föregående BMT-fösöket i Stripa att vara tillhängliga.

Det föreliggande dokumentet ger en summering av de viktigaste dragen hos modellerna utan någon värdering.

3. CONCEPTUAL BUFFER MODEL

General

The development of THMCB models should be based on an understanding of the physico/chemical processes that will take place in the buffer at different stages. Figure 2-1 shows the interacting components.

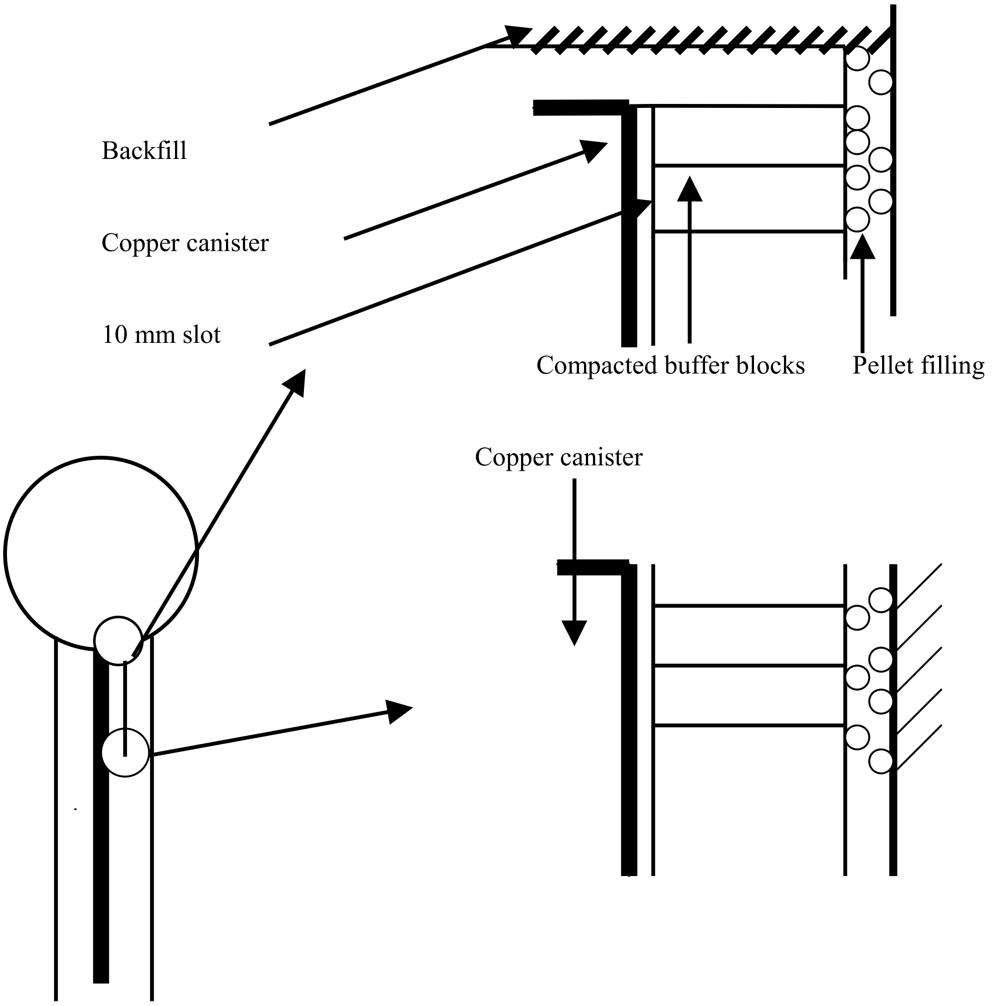

Figure 2-1. *KBS3 deposition hole with copper-shielded canister embedded in compacted buffer blocks and bentonite pellet filling.*

Redistribution of intially contained porewater in the buffer

A number of physico/chemical events will take place in the maturation of the buffer of which the following are considered to be particularly important:

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. Dissolution of buffer minerals and precipitation of chemical compounds in the buffer

The main consequences of the water redistribution are:

a) The heat conductivity of the inner part of the buffer clay is decreased while the outer part becomes more heat-conductive.

b) The outer, wetted part expands and undergoes some drop in dry density while the inner part shrinks and fractures.

Maturation of the 50 mm thick pellet backfill with homogenisation and consolidation under the swelling pressure exerted by the hydrating and expanding blocks

The intial 50 mm slot filled with pellets and water is consolidated by the expanding buffer blocks, which take up water from the filling and also from the rest of the blocks by migration of water from the hot parts to the colder, outer part. One can identify four main processes: i) expansion of the pellets and homogenization of the pellet filling, ii) water uptake and expansion of the buffer blocks, and iii) compression of the pellet filling. The first process (i) is probably completed before ii) and iii) become important and can be treated separately, while the other two are coupled inverse functions. It is assumed that these latter processes take place parallel to the uptake of water from the rock except in very tight rock.

The process has a B-effect implying that microbes can enter the pellet filling and survive and multiplicate until the density of the filling has apporoached 1600 kg/m^3.

The major consequences of the maturation of the pellet filling are:

a) The hydraulic conductivity of the outermost part of the buffer drops and the inflow of water from the rock into the deposition holes decreases

b) There is competition with respect to water between the densifying pellet filling and the softening buffer blocks.

Uptake of water from the rock

Uptake of water from the rock and backfill is the THMC process that ultimately yields complete water saturation and the ultimate 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 at the contact between buffer and backfill may rise relatively quickly if it is supplied with water from intersected hydraulically active fracture zones but may otherwise be rather low.

The rock around the deposition holes gives off water through discrete hydraulically and mechanically active or activized discontinuities. The hydraulic transport capacity 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 the intersecting fractures and by the conductivity of the shallow boring-disturbed zone (EDZ).

The hydration of the buffer and backfill by uptake of water from the rock is associated with expansion of the upper part of the buffer and consolidation of the backfill as well as with axial displacement of the canisters due to altered rheological properties of the moistening buffer.

The wetting has a C-effect since Ca^{2+}, Mg^{2+}, K^{+}, SO_4^{-2} and Cl^{-} will be precipitated at the wetting front which moves towards the canister. A rather large part of the buffer may hence contain such precipitates and interact with the smectite minerals and the copper canister. The temperature gradient has a C-effect since silicate minerals including the smectite component will dissolve to a larger extent close to the heater than close to the rock by which released silica migrates towards the rock and precipitates in the outer part of the bentonite. The silification causes some cementation and brittleness of the clay. Minerals with reversed solubility, like sulphates and carbonates, will be precipitated in the hottest part where some cementation will also take place.

The major consequences of the water uptake are:

a) Water uptake from the backfill and rock gives the desired condition of the canisters being completely embedded by a practically impermeable clay medium. Its physical properties may be affected by ion exchange

b) The canister may undergo displacement in the course of the wetting of the buffer

c) Expansion of the upper part of the buffer and compression of the contacting backfill changes their hydraulic conductivities. Shearing of hydraulically active rock discontinuities may have an impact on the ability of the rock to give off water to the deposition holes

d) The rate of water uptake enhances salt precipitation in the buffer close to the canisters and corrosion of the copper canisters.

4. WHAT IS MEASURED IN THE PROTOTYPE REPOSITORY?

The processes measured in the Prototype Repository Project 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. Water chemistry.

One finds that 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. The models can be improved and calibrated by use of the recordings and it is expected that this will improve them and show limitations and possibilities.

5. EBS MODEL CODES

4.1 CODE "COMPASS", H.R Thomas and P.J Cleall, Cardiff University

4.1.1 Introduction

COMPASS (**CO**de for **M**odelling **PA**rtly **S**aturated **S**oil) is based on a mechanistic theoretical formulation, where the various aspects of soil behaviour under consideration, are included in an additive manner. In this way the approach adopted describes heat transfer, moisture migration, solute transport and air transfer in the material, coupled with stress/strain behaviour.

4.1.2 General description of formulation employed

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

The main features of the formulation are described below.

- 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.

4.1.3 Theoretical Formulation

Heat transfer

Conservation of energy is defined according to the following classical equation:

$$\frac{\partial \Omega_H}{\partial t} = -\nabla.\mathbf{Q} \qquad (1)$$

where Ω_H, the heat content of the partly saturated soil per unit volume is defined as:

$$\Omega_H = H_c\left(T - T_r\right) + LnS_a\rho_v$$

T is the temperature, T_r the reference temperature, H_c the heat capacity of the party saturated soil, L is the latent heat of vaporisation, n is the porosity, S_a is the degree of saturation with respect to the air phase and ρ_v is the density of the water vapour.

Following the approach presented by Ewen and Thomas (1989) the heat capacity of unsaturated soil H_c at the reference temperature, T_r, can be expressed as:

$$H_c = (1-n)C_{ps}\rho_s + n\left(C_{pl}S_l\rho_l + C_{pv}S_a\rho_v + C_{pda}S_a\rho_{da}\right) \qquad (2)$$

where C_{ps}, C_{pl}, C_{pv} and C_{pda} are the specific heat capacities of solid particles, liquid, vapour and dry air respectively, ρ_s is the density of the solid particles, ρ_{da} is the density of the dry air, ρ_l is the density of liquid water and S_l the degree of saturation with respect to liquid water.

The heat flux per unit area, **Q**, can be defined as (Thomas and King, 1991):

$$\mathbf{Q} = -\lambda_T\nabla T + \left(\mathbf{v_v}\rho_v + \mathbf{v_a}\rho_v\right)L + \left(C_{pl}\mathbf{v_l}\rho_l + C_{pv}\mathbf{v_v}\rho_l + C_{pv}\mathbf{v_a}\rho_v + C_{pda}\mathbf{v_a}\rho_{da}\right)\left(T - T_r\right) \qquad (3)$$

where λ_T is the coefficient of thermal conductivity of the partly saturated soil and $\mathbf{v_l}$, $\mathbf{v_v}$ and $\mathbf{v_a}$ are the velocities of liquid, vapour and air respectively.

The governing equation for heat transfer can be expressed, in primary variable form as:

$$C_{Tl}\frac{\partial u_l}{\partial t} + C_{TT}\frac{\partial T}{\partial t} + C_{Ta}\frac{\partial u_a}{\partial t} + C_{Tu}\frac{\partial \mathbf{u}}{\partial t} = \nabla.\left[K_{Tl}\nabla u_l\right] + \nabla.\left[K_{TT}\nabla T\right] + \nabla.\left[K_{Ta}\nabla u_a\right] + V_{Tl}\nabla u_l + V_{TT}\nabla T + V_{Ta}\nabla u_a + V_{Tc_s}\nabla c_s + J_T \qquad (4)$$

where C_{Tj}, V_{Tj}, K_{Tj} and J_T are coefficients of the equation (j = l, T, a, c_s, $\boldsymbol{u}$), and $\boldsymbol{u}$ is a deformation vector.

Moisture transfer

The governing equation for moisture transfer in a partly saturated soil can be expressed as:

$$\frac{\partial(\rho_l n S_l)}{\partial t} + \frac{\partial(\rho_v n(S_l - 1))}{\partial t} = -\rho_l \nabla.\mathbf{v_l} - \rho_l \nabla.\mathbf{v_v} - \nabla.\rho_v \mathbf{v_a} \tag{5}$$

where *t* is the time. The velocities of pore liquid and pore air are calculated using a generalised Darcy's law, as follows

$$\mathbf{v_l} = -K_l\left(\nabla\left(\frac{u_l}{\gamma_l}\right) + \nabla z\right) + K_l^{c_s}(\nabla c_s) \tag{6}$$

$$\mathbf{v_a} = -K_a \nabla u_a \tag{7}$$

where K_l is the hydraulic conductivity, $K_l^{c_s}$ is the hydraulic conductivity with respect to chemical solute concentration gradient, K_a is the conductivity of the air phase, γ_l is the specific weight of water, u_l is the pore water pressure, *z* is the elevation, u_a is the pore air pressure and c_s the chemical solute concentration.

The inclusion of an osmotic flow term in the liquid velocity allows the representation of liquid flow behaviour found in some highly compacted clays, (Yong and Warkentin, 1966; Yong and Warkentin, 1975). The definition of vapour velocity follows the approach presented by Thomas and King (1991) which was based on the flow law proposed by Philip and de Vries (1957). The governing equation for moisture transfer can be expressed, in primary variable form as:

$$C_{ll}\frac{\partial u_l}{\partial t} + C_{lT}\frac{\partial T}{\partial t} + C_{la}\frac{\partial u_a}{\partial t} + C_{lu}\frac{\partial \mathbf{u}}{\partial t} = \nabla.[K_{ll}\nabla u_l] + \nabla.[K_{lT}\nabla T] + \nabla.[K_{la}\nabla u_a] + \nabla.[K_{lc_s}\nabla c_s] + J_l \tag{8}$$

where C_{lj}, K_{lj} and J_l are coefficients of the equation ($j = l, T, a, c_s, \mathbf{u}$).

Dry air transfer

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 contained in the pore liquid is defined using Henry's law.

$$\frac{\partial[S_a + H_s S_l]n\rho_{da}}{\partial t} = -\nabla.[\rho_{da}(\mathbf{v_a} + H_s \mathbf{v_l})] \tag{9}$$

where H_s is the coefficient of solubility of dry air in liquidisation.

The governing equation for dry air transfer can be expressed, in primary variable form as:

$$C_{al}\frac{\partial u_l}{\partial t}+C_{aT}\frac{\partial T}{\partial t}+C_{aa}\frac{\partial u_a}{\partial t}+C_{au}\frac{\partial \mathbf{u}}{\partial t}=\nabla.[K_{al}\nabla u_l]+\nabla.[K_{aa}\nabla u_a]+\nabla.[K_{ac_s}\nabla c_s]+J_a \tag{10}$$

where C_{aj}, K_{aj} and J_a are coefficients of the equation ($j = l, T, a, c_s, \mathbf{u}$).

Chemical solute transfer

Where a chemical solute is considered non-reactive and sorption onto the soil surface is ignored the governing equation for conservation of chemical solute can be defined as (Bear and Verruijt, 1987):

$$\frac{\partial(nS_l c_s)}{\partial t}=-\nabla.[c_s\mathbf{v}_1]+\nabla.[D_h\nabla(nS_l c_s)] \tag{11}$$

where D_h is the hydrodynamic dispersion coefficient defined as (Bear and Verruijt, 1987):

$$D_h = D + D_d \tag{12}$$

D_h includes both molecular diffusion, D_d, and mechanical dispersion, D.

The governing equation for chemical solute transfer can be expressed, in primary variable form as:

$$C_{c_sl}\frac{\partial u_l}{\partial t}+C_{c_sa}\frac{\partial u_a}{\partial t}+C_{c_sc_s}\frac{\partial c_s}{\partial t}+C_{c_su}\frac{\partial \mathbf{u}}{\partial t}=\nabla.[K_{c_sl}\nabla u_l]+\nabla.[K_{c_sT}\nabla T]+ \\ \nabla.[K_{c_sa}\nabla u_a]+\nabla.[K_{c_sc_s}\nabla c_s]+J_{c_s} \tag{13}$$

where C_{c_sj}, K_{c_sj} and J_{c_s} are coefficients of the equation ($j = l, T, a, c_s, \mathbf{u}$).

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 suitable geochemical model.

Stress-strain relationship

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

$$d\varepsilon = d\varepsilon_\sigma + d\varepsilon_{c_s} + d\varepsilon_s + d\varepsilon_T \tag{14}$$

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 equation **Fel! Hittar inte referenskälla.**. 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 described the contribution of the chemical solute via a elastic relationship based on osmotic potential.

The governing equation for stress-strain behaviour can be expressed, in primary variable form as:

$$C_{ul}du_l + +C_{uT}dT + C_{ua}du_a + C_{uc_s}dc_s + C_{uu}d\mathbf{u} + d\mathbf{b} = 0 \qquad (15)$$

where C_{uj} *are* coefficients of the equation ($j = l$, T, a, c_s, $\boldsymbol{u}$) and **b** is the vector of body forces.

4.1.4 Numerical solution

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.

<u>*Spatial discretisation*</u>

The Galerkin weighted residual method is employed to formulate the finite element discretisation. For the flow equations a shape function N_m is used to define an approximation polynomial:

The general flow equation

$$\frac{\partial M}{\partial t} + \nabla.\underline{q} = 0 \qquad (16)$$

where M refers to mass or enthalpy and $\underline{q}$ refers to the flux term, can be discretised via the Galerkin method as:

$$\int_{\Omega}\left(N_m^t\frac{\partial M}{\partial t} + \nabla N_m^t.\underline{q}\right)d\Omega + \int_{\Gamma_1} N_m^t.\underline{q}^* d\Gamma = 0 \qquad (17)$$

where $\underline{q}^*$ is a flux prescribed at boundary Γ_1.

The same method can be applied to the stress equilibrium equation, which with the use of a shape function N_f, yields:

$$\int_{\Omega} \left(\mathbf{B}^t \mathbf{D}\left(\mathbf{B}du + \mathbf{A_s}du_l - \mathbf{A_s}du_a - \mathbf{A}_{c_s}dc_s - \mathbf{A_s}dT\right)\right)d\Omega - \int_{\Gamma_1} N_f^T\left(\nabla du_a + db_i\right)d\Omega - \int_{\Gamma_1} N_f^T \underline{\tau} d\Gamma = 0$$

(18)

where **B** is the strain matrix and $\underline{\tau}$ is the surface traction.

Applying this methodology to the governing differential equations, yields, in matrix form:

$$\begin{bmatrix} \mathbf{K_{ll}} & \mathbf{K_{lT}} & \mathbf{K_{la}} & \mathbf{K_{lC_s}} & \mathbf{0} \\ \mathbf{K_{Tl}} & \mathbf{K_{TT}} & \mathbf{K_{Ta}} & \mathbf{K_{TC_s}} & \mathbf{0} \\ \mathbf{K_{al}} & \mathbf{0} & \mathbf{K_{aa}} & \mathbf{K_{aC_s}} & \mathbf{0} \\ \mathbf{K_{C_sl}} & \mathbf{K_{C_sT}} & \mathbf{K_{C_sa}} & \mathbf{K_{C_sC_s}} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} u_l \\ T \\ u_a \\ c_s \\ \underline{u} \end{bmatrix} + \begin{bmatrix} \mathbf{C_{ll}} & \mathbf{C_{lT}} & \mathbf{C_{la}} & \mathbf{C_{lC_s}} & \mathbf{C_{lu}} \\ \mathbf{C_{Tl}} & \mathbf{C_{TT}} & \mathbf{C_{Ta}} & \mathbf{C_{TC_s}} & \mathbf{C_{Tu}} \\ \mathbf{C_{al}} & \mathbf{C_{aT}} & \mathbf{C_{aa}} & \mathbf{C_{aC_s}} & \mathbf{C_{au}} \\ \mathbf{C_{C_sl}} & \mathbf{C_{C_sT}} & \mathbf{C_{C_sa}} & \mathbf{C_{C_sC_s}} & \mathbf{C_{C_su}} \\ \mathbf{C_{ul}} & \mathbf{C_{uT}} & \mathbf{C_{ua}} & \mathbf{C_{uC_s}} & \mathbf{C_{uu}} \end{bmatrix} \begin{bmatrix} \dot{u}_l \\ \dot{T} \\ \dot{u}_a \\ \dot{c}_s \\ \underline{\dot{u}} \end{bmatrix} + \begin{bmatrix} f_l \\ f_T \\ f_a \\ f_{c_s} \\ f_u \end{bmatrix} = 0$$

(19)

where $\mathbf{K_{ij}}$ and $\mathbf{C_{ij}}$ represent the corresponding matrices of the governing equation (i,j=l,T,a,c_s,u).

Equation (19) can be rewritten, in a more concise notation, as:

$$\mathbf{A}\phi + \mathbf{B}\frac{\partial \phi}{\partial t} + \mathbf{C} = \{0\} \qquad (20)$$

where ϕ represents the variable vector $\{u_l, T, u_a\ c_s, \boldsymbol{u}\}^t$.

Temporal discretisation

To solve equation (4-21) a numerical technique is required to achieve temporal discretisation. In this case an implicit mid-interval backward difference algorithm is implemented since it has been found to provide a stable solution for highly non-linear problems (Thomas and King, 1991). This can be expressed as:

$$\mathbf{A}^{n+\frac{1}{2}}\phi^{n+1} + \mathbf{B}^{n+\frac{1}{2}}\left[\frac{\phi^{n+1} - \phi^{n}}{\Delta t}\right] + \mathbf{C}^{n+\frac{1}{2}} = \{0\} \qquad (21)$$

where the superscript represents the time level (the superscript *n* represents the last time interval and *n+1* represents the time level where the solution is being sought). Rearrangement of equation 21 yields:

$$\boldsymbol{\phi}^{n+1} = \left[\mathbf{A}^{n+\frac{1}{2}} + \frac{\mathbf{B}^{n+\frac{1}{2}}}{\Delta t}\right]^{-1} \left[\frac{\mathbf{B}^{n+\frac{1}{2}}\boldsymbol{\phi}^{n}}{\Delta t} - \mathbf{C}^{n+\frac{1}{2}}\right] \qquad (22)$$

A solution can be found to equation (23) if **A, B** and **C** can be evaluated. This is achieved via an iterative scheme. For each iteration a revised set of **A, B** and **C** are calculated and the resulting solution checked for convergence against the following criteria:

$$\left|\frac{\boldsymbol{\phi}_{i}^{n+1} - \boldsymbol{\phi}_{(i-1)}^{n+1}}{\boldsymbol{\phi}_{(i-1)}^{n+1}}\right| \quad \mathbf{TL}_{rel} \qquad (23)$$

where $\mathbf{TL}_{\mathrm{rel}}$ is the relative tolerance and *i* represents the iteration level. Successive iterations are performed until this criteria is satisfied.

With appropriate initial and boundary conditions the set of non-linear coupled governing differential equations can be solved via the numerical solution presented above.

4.1.5 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’.

The pre and post processor is a Microsoft Windows graphic user interface (GUI) written in VISUAL BASIC. The GUI allows the definition of problems (including geometry, material parameters, initial conditions and boundary conditions), the generation of finite element meshes and the display of results as contour plots, mesh displacement animations and x-y profiles.

The engine, written in FORTRAN 90, is a modularly structured finite element analysis programme. An extensive library of finite elements is included which allows 1D, 2D plane, 2D axisymmetric and 3D geometry problems to be analysed.

Use of the well-established time stepping scheme described in section 4 allows both steady state and transient problems to be analysed. This time stepping scheme is implemented with a variable timestep algorithm to provide an efficient solution. The number of iterations required for convergence is related to the size of the time step used. This property is used to modify the time step size employed as a simulation progresses. If the number of iterations exceeds a specified value, the time step size is reduced by a factor. Likewise, if the number of iterations required falls below a specified value, the time step size is increased by a specified factor.

Evaluation of integrals is achieved via Gaussian integration. For the elasto-plastic based stress equilibrium equations a stress return algorithm is required. A backward Euler procedure is employed (Crisfield, 1991) with the tangent cutting method (Ortiz and Simon, 1986) used to improve the accuracy of this algorithm. Both direct and indirect solution methods are available to solve the set of simultaneous equations including frontal, LU, LDLT, Cholesky and a number of conjugate gradient and preconditioner solvers (Hinton and Owen, 1977; Bathe, 1996).

Extensive use of COMPASS over a period of years has served to illustrate the robustness of the numerical scheme.

4.1.6 Verification

Additionally, also over a period of years, verification and validation exercises have been performed on COMPASS. These include both in-house and independent programmes (Thomas and Li, 1997, Thomas et al, 1998). The verification programme has consisted of an extensive series of checks against:

- analytical solutions where such solutions exist – e.g. Carlsaw and Jaegar (1959) for flow phases
- single point calculations – e.g. Integration over load paths to verify development of strain
- numerical solutions from other computer codes, developed independently of COMPASS – e.g. Comparison of 3D heat flow problems with proprietary heat flow software.

4.1.7 Validation

The validation program has aimed to carry out a series of checks, this time against well-controlled experimental work. The programme has attempted to validate components of the formulation in a 'step by step' manner:

- Heat transfer alone
- Isothermal moisture movement alone
- Coupled heat and moisture movement (Thomas and Li, 1997)
- Coupled moisture and air movement (Thomas and Sansom, 1995)
- Coupled heat, moisture and deformation for slightly swelling clay (Thomas and He, 1995, Thomas and He, 1998)
- Coupled heat, moisture and deformation in the CATSIUS CLAY Project.

It is recognised, however, that validation of the code is a process rather than a series of events. As such, continued work on this aspect is envisaged. In particular further exploration of the validation of the mechanical components of the formulation, especially for highly swelling soils, is considered to be essential. The work performed so far is quoted however as an illustration of the confidence gained to date in the ability of the code to reproduce physically observed behaviour.

4.1.8 Numerical solution, Applications – relevant to the high level nuclear waste repository problem

COMPASS has been applied to a large number of problems. In particular for the HLW repository problem the following exercises have been carried out:

- Simulation of in-situ test BACCHUS 1 carried out at SCK/CEN's URL
- Simulation of in-situ test BACCHUS 2 carried out at SCK/CEN's URL
- Simulation of small scale infiltration tests on Boom clay
- Simulation of AECL's isothermal in-situ test
- Simulation of AECL's buffer container experiment
- Simulation of AECL's in-room emplacement scenario
- Simulation of various small scale heating tests carried out by CIEMAT
- Simulation of the FEBEX mock-up test

4.1.9 Numerical solution, Description of the processes involved in the simulation of the Prototype Repository, which can be modelled by COMPASS

To illustrate the capability of the code, this section details the various stages of the simulation of the prototype repository that can be modelled using COMPASS. For each stage, the process addressed and the boundary conditions required will be detailed. Geometry and boundary conditions already specified in preceding stages will not be repeated.

Excavation process

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 Excavation Damaged Zone (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.

Equalisation stage

This covers the period after placement of the canisters, buffer, pellets and water and prior to activation of the heaters. Processes to be addressed include the hydration of the buffer from the pellet region and subsequent swelling of buffer and softening of the pellet region. Initial stages of equalisation of the rock mass with the emplaced material are also included. Depending on the expected time for the homogenisation of the pellet and water mix to a homogenous gel, the maturation process of the pellets can be addressed either as a coupled problem or an uncoupled problem. It is probable that the process will be completed before the other processes in this stage become important and therefore the pellet region can be treated as a homogenous material. Boundary conditions required include: geometry of canister, buffer, backfill and pellet region; duration of equalisation stage; initial conditions of buffer, backfill and pellet gel.

Heating and resaturation stage

This covers the period after the heaters in the canisters are activated. Processes to be addressed include: the flow of heat due to conduction, convection and latent heat of vapourisation; redistribution of moisture field due to thermal loading, including the flow of vapour and moisture due to thermal and potential gradients; the effect of redistribution of moisture content on thermal regime; the development of stress-strain field due to changes in hydraulic and thermal fields. Boundary conditions required include details of heating regime.

4.1.10 Numerical solution, Material parameters

A set of material parameters are required for each of the following materials i) rock mass, ii) excavation damaged zone in the granite rock mass, iii) buffer, iv) backfill, v) pellet gel.

The parameters required for each material can be considered in three groups, as follows:

Hydraulic parameters: These include: initial porosity, saturated hydraulic conductivity, unsaturated hydraulic conductivity, Water retention relationship, unsaturated air and vapour flow parameters.

Thermal parameters: These include: thermal conductivity, specific heat capacity of soil solid and density of soil.

Mechanical parameters: These are listed as follows: shear modulus, elastic stiffness (stress), plastic stiffness (stress), reference stress, preconsolidation stress, hardening parameter of si, elastic stiffness (suction)plastic stiffness (suction), parameter for cohesion hardening, parameter for ramd(s), slope of critical state line, coefficient of thermal expansion.

4.1.11 Numerical solution, Limitations of the approach

Some issues to be considered in relation to limitations of the approach are listed below:

i) The modelling approach is based on a mechanistic formulation. Hence there is a need for validation at all stages to ensure that the physical chemical processes are correctly represented. For example, for the vapour flow processes in densely compacted clays there is currently a limited availability of data. Also, the stress-strain models employed in the THM modelling work are based on conventional partly saturated soil constitutive models, for example elasto-plastic suction based approach. Applicability of such models to highly swelling densely compacted clay merits further investigation. Finally, THCM behaviour is modelled via coupling with a Geochemical code. Again complexities of bentonite behaviour requires careful consideration.

ii) There is only limited experimental data available to define parameters. Further experimental work is necessary in support of this aspect.

iii) Large scale simulations, as envisaged here, are potentially very computationally demanding.

4.1.12 Example

<u>Generic repository</u>

The descriptive example investigated here involves the placement of a full-size heater in a 5m deep borehole with a bentonitic buffer material (Figure 4-1). 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.

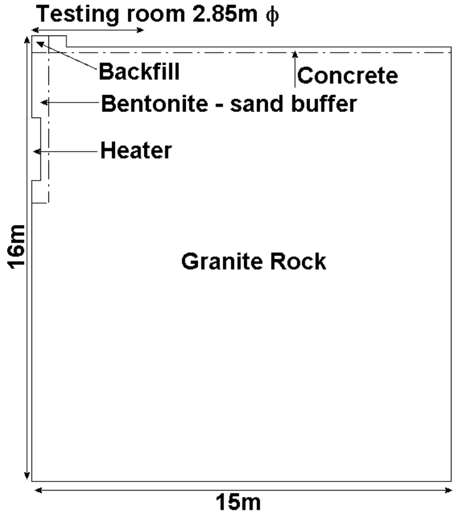

Figure 4-1. *Axisymmetric domain.*

Thermal conditions

An initial rock temperature of 11°C was taken with an average air temperature of 15°C within the tunnels and caverns. At the start of the heating phase a constant power of 1000W was applied to the heater. After 26 days the power to the heater was increased to 1200W in order to reach the required heater temperature of 85°C.

Numerical modelling

A 15m by 16m axisymmetric domain shown in Figure 4-1 was adopted, and discretised with 1165, 8-noded, isoparametric, finite elements. 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 showed that during the dwell period desaturation occured within the rock for a distance of approximately 1.5m from the centre of the heater. Finally the heating stage was addressed via a coupled temperature and mass analysis. The results for 210 days of heating are shown in Figure 4-2. The effect of the varying value of thermal conductivity, due both to the different materials and the effect of drying near to the heater, can be clearly seen with distinct changes of gradient in the temperature profile.

Results for the pore water pressures during the heating period are shown in Figure 4-3. It can be seen that in the numerical results the pore water pressure is still increasing after 200 days and the results have not yet peaked.

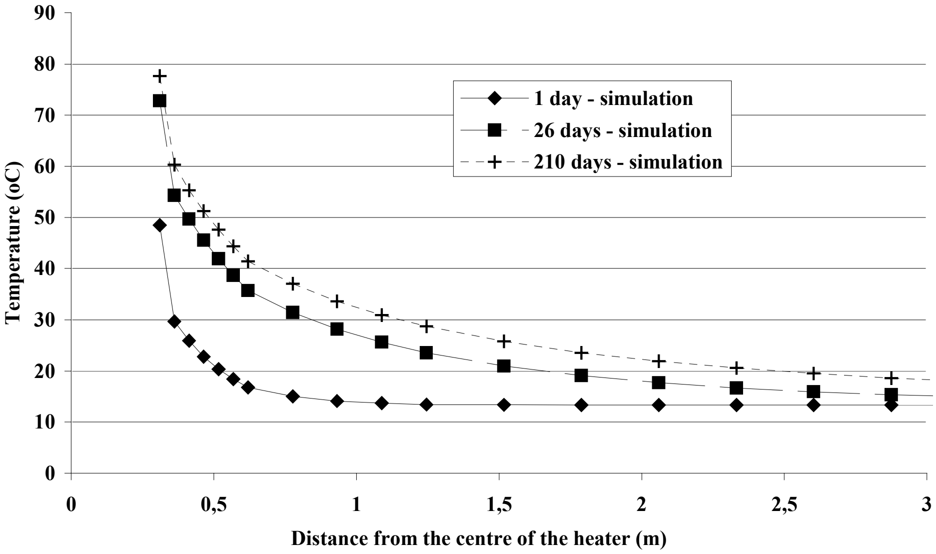

***Figure 4-2**: Temperature distributions along the mid-height of the heater*

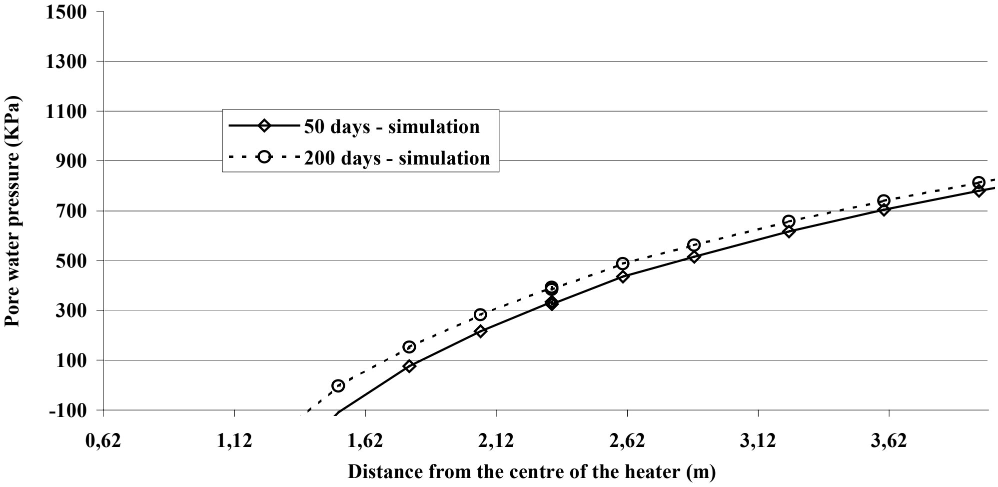

***Figure 4-3:** Pore water pressure profiles with time during the heating period.*

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4.2 CODE "BRIGHT", A. Ledesma, CIMNE (ENRESA)

4.2.1 Introduction

The CODE BRIGHT is a finite element code for the analysis of THM problems in geological media that has been developed by the Geomechanics group of the Geotechnical Engineering and Geosciences Departament, Technical University of Catalunya – Center for Numerical Methods in Engineering (UPC-CIMNE, Barcelona, Spain).

4.2.2 Basic approach

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 1, the problem is formulated in a multiphase and multispecies approach.

The three phases are

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

The three species are:

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

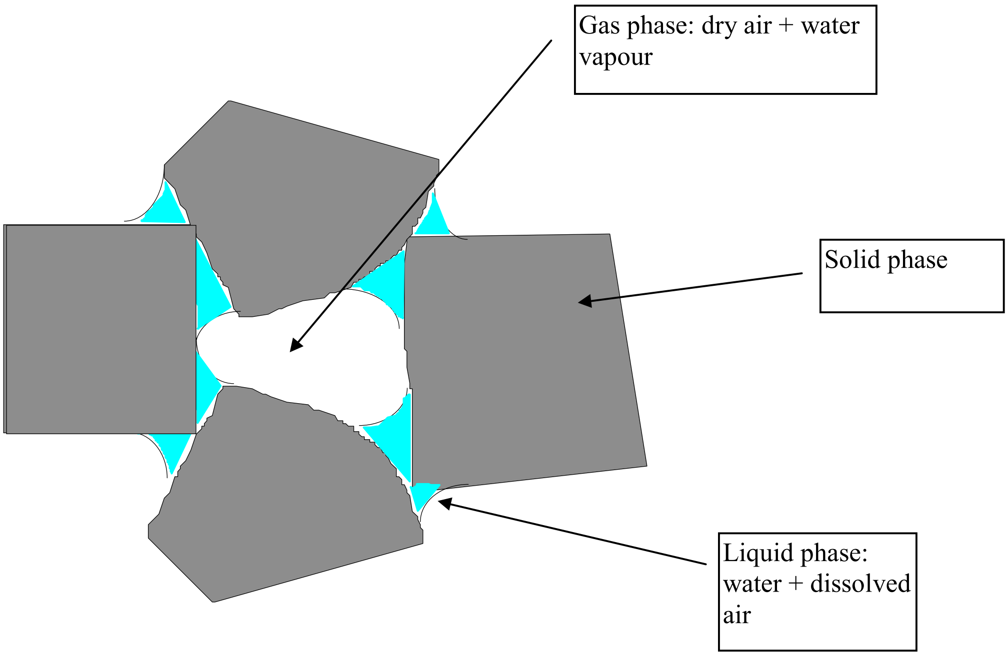

Figure 4-4. *Schematic representation of an unsaturated porous material.*

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

- Dry air is considered a single species and it 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, $\boldsymbol{u}$ (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:

Mass balance of solid
Mass balance of water
Mass balance of air
Momentum balance for the medium
Internal energy balance for the medium

Associated with this formulation there is a set of necessary constitutive and equilibrium laws. Table 4-1 is a summary of the constitutive laws and equilibrium restrictions that have been incorporated in the general formulation. The dependent variables that are computed using each laws are also included.

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. The governing equations are finally written in terms of the unknowns (indicated in Table 4-2) when the constitutive equations are substituted in the balance equations.

Table 4-1. 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

Table 4-2. Equations and summary of variables.

Equation	Variable name	Variable
Equilibrium of stresses	displacements	$\mathbf{u}$
Balance of water mass	liquid pressure	P_l
balance of air mass	gas pressure	P_g
Balance of internal energy	temperature	T

The resulting system of PDE's (Partial Differential Equations) is solved numerically. The numerical approach can be viewed as divided into two parts: spatial and temporal discretizations. Finite element method is used for the spatial discretization while finite differences are used for the temporal discretization. The discretization in time is linear and the implicit scheme uses two intermediate points, $t^{k+\varepsilon}$ and $t^{k+\theta}$ between the initial t^k and final t^{k+1} times. Finally, since the problems are non-linear, the Newton-Raphson method has been adopted to find an iterative scheme. The main features of the numerical approach are indicated in Table 4-3, and the general features of the Code in Table 4-4.

Table 4-3. Numerical features of Code Bright

Concept	Description	Comments
Elements	Segments, triangles, quadrilaterals, quadratic triangles, tetrahedrons, triangular prisms, quadrilateral prisms.	Axisymetry option
Integration	Analytical integration is used for segments, triangles and tetrahedrons. Numerical integration for the other.	Influence coefficients strategy.
Time-marching	Finite differences and implicit scheme are used for time integration. Two intermediate points: ($t^{k+\theta}$) and ($t^{k+\varepsilon}$).	For instance $\varepsilon=0$ (lin.) and $\theta=1$ (fully implicit).
Non-linear	Newton-Raphson method for solution of the non-linear system of algebraic equations that results once the space and time discretizations are applied.	All equations solved together. Safest method.
System of equations	LU decomposition and backsubstitution or conjugate gradients (iterative). (non symmetric matrix).	Band storage or compressed sparse, resp.
Time stepping	Automatic discretization of time. Increase or reduction of time step according to convergence conditions. Reduction of time increment may be caused by: large variation of unknowns per iteration, large number of iterations to reach convergence and error increase.	Tolerances for each criterium are user defined.

Table 4-4. Main general features of CODE BRIGHT.

Concept	Description
Options	– Allow to solve uncoupled and coupled problems. – For instance: M, H, T, HM, TM, TH, THM.
Types of analyses	– One dimension (uni-axial confined strain and axi-symmetric). – Two dimension (plane strain and axi-symmetric). – Three dimensions
Constitutive laws	– Each law defined as a set of parameters (from 1 parameter to several).
Boundary conditions	– Mechanical problem: forces and displacement rate in any spatial direction. – Hydraulic problem: mass flow rate of water and air prescribed and liquid/gas pressure prescribed. – Thermal problem: heat flow rate prescribed and temperature prescribed.
Convergence criteria	– Tolerances for absolute and relative error independent for each unknown. Tolerance for residual convergence of each problem (mechanical, hydraulic, etc).
Output options	– Spatial distribution of variables at user defined time points – Time evolution of variables at user defined space points

4.2.3 Description of the work

CIMNE-UPC participates in the following activities:

- T and TM modelling
- HM and THM modelling of rock mass
- THM modelling of buffer, backfill and interaction with near-field rock
- C modelling of buffer, backfill and groundwater

The most complex analysis is the THM modelling of the canister – bentonite – pellets - near rock materials because of the couplings between the thermal and the hydraulic problem. Figure 4-5 shows those couplings in a simplified manner. If the vapour transport is considered in detail, then the couplings can incorporate gas advection as well. The equations involved were indicated in Table 4-1.

The mechanical stress-strain relationship of the bentonite will be defined by means of an elastoplastic model specially designed for unsaturated soil behaviour (known as the "Barcelona Basic Model") – see reference 3 -. Differences between the zone with pellets and the blocks of bentonite will probably be considered during early times by means of different parameters, using the same model. Rock will be considered elastic in all the analyses.

An attempt to simulate the THMC problem will be carried out as well, including reactive transport in the problem. In this case, considering the amount of variables involved, a 1D analysis is expected to be done, studying only one deposition hole and assuming axisymmetric geometry. One boundary will be the heater, and the other one the rock. CODE BRIGHT is already prepared to deal with this case (see reference 4, at the beginning of the presentation), although is still being improved regarding the chemical problem. The type of processes to be considered can include complex formation, oxidation/reduction reactions, acid/base reactions, precipitation/dissolution of minerals, cation exchange, sorption and radioactive decay. The total analytical concentrations are adopted as basic transport variables and chemical equilibrium is achieved by minimizing Gibbs Free Energy.

The THMC approach will be adopted at the end of the project, and simple constitutive equations for the mechanical part of the problem will be adopted. This is to keep under reasonable values the computing time of the problem. Also the analysis will focus on the chemical effects, specially coupled to the thermal and hydraulic problems.

4.2.4 Example

As an example, a preliminary analysis of a part of the Prototype Geometry is presented. It is a TH analysis considering all the couplings indicated, and assuming the parameters corresponding to the MX80 bentonite and to the rock available in the literature and in the SKB reports. For the pellets, a variation of the bentonite parameters has been adopted. The behaviour of the pellets will require additional analyses in the future, because of their special characteristics and the difficulties when simulating their behaviour.

A 2D analysis of two deposition holes (their cross-section) has been performed. Figure 4-5 presents the evolution of temperature along time, and Figure 4-6 shows that evolution for the degree of saturation. Note that bentonite becomes practically saturated in about 5 months. This is of course a preliminary result, and should be confirmed in further analyses with different parameters. Finally, Figures 4-7 and 4-8 present contours of temperature and degree of saturation at 365 and 33 days respectively.

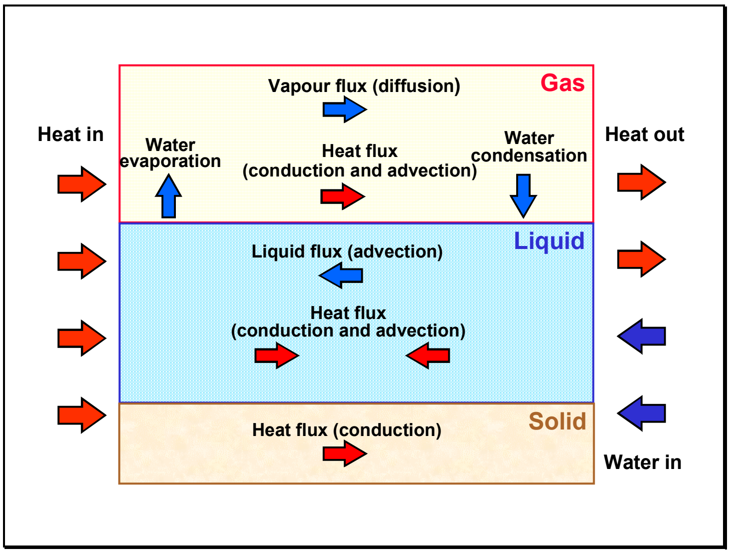

Figure 4-5. *Main couplings considered in the TH problem.*

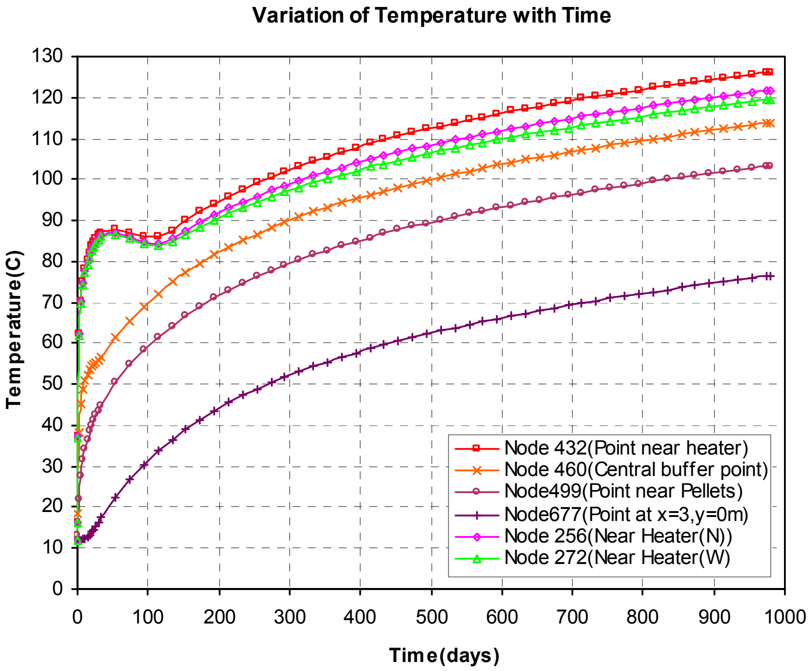

Figure 4-6. *Temperature vs. Time for different points*

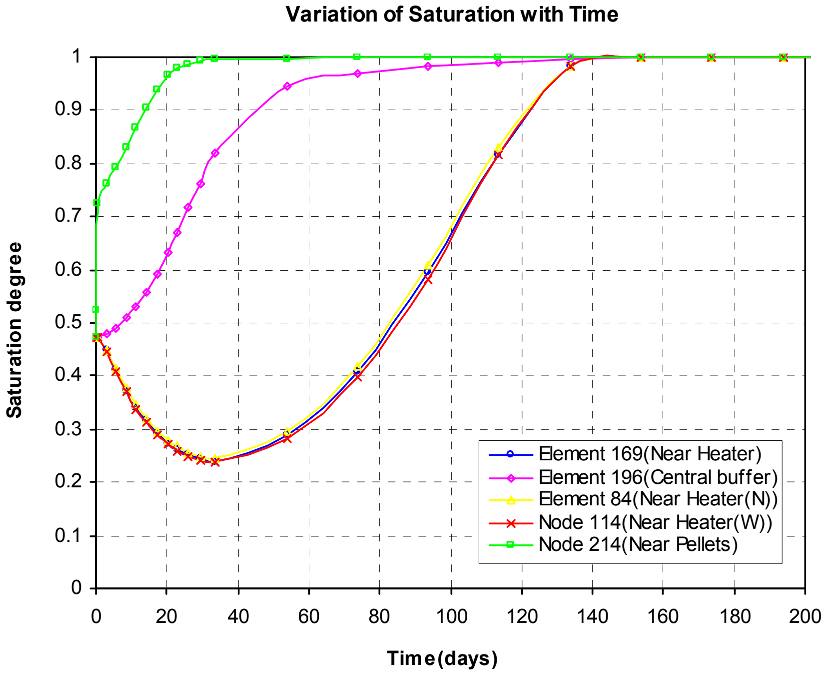

Figure 4-7. *Degree of saturation vs. Time for different points*

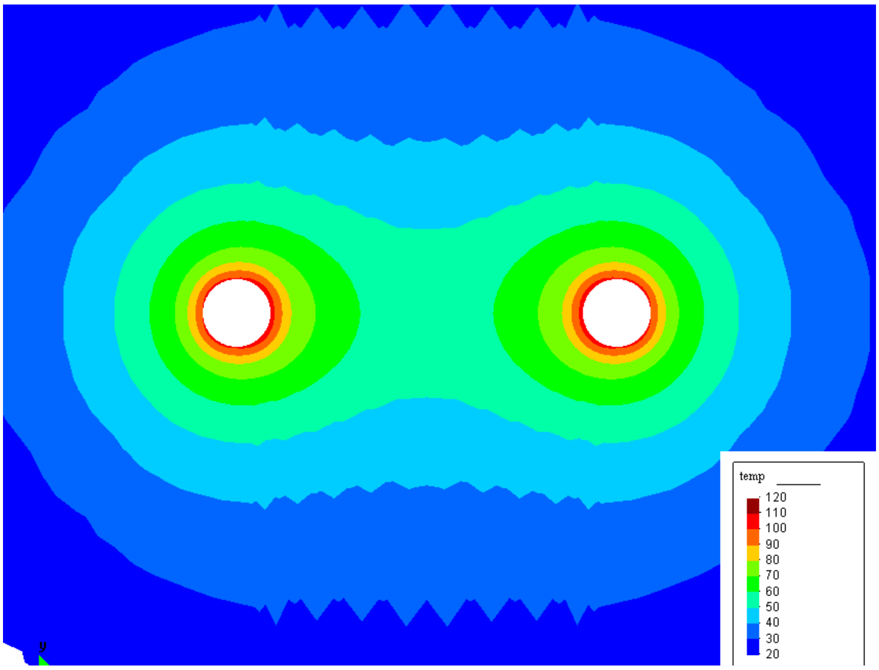

Figure 4-8. *Temperature contour after1 year.*

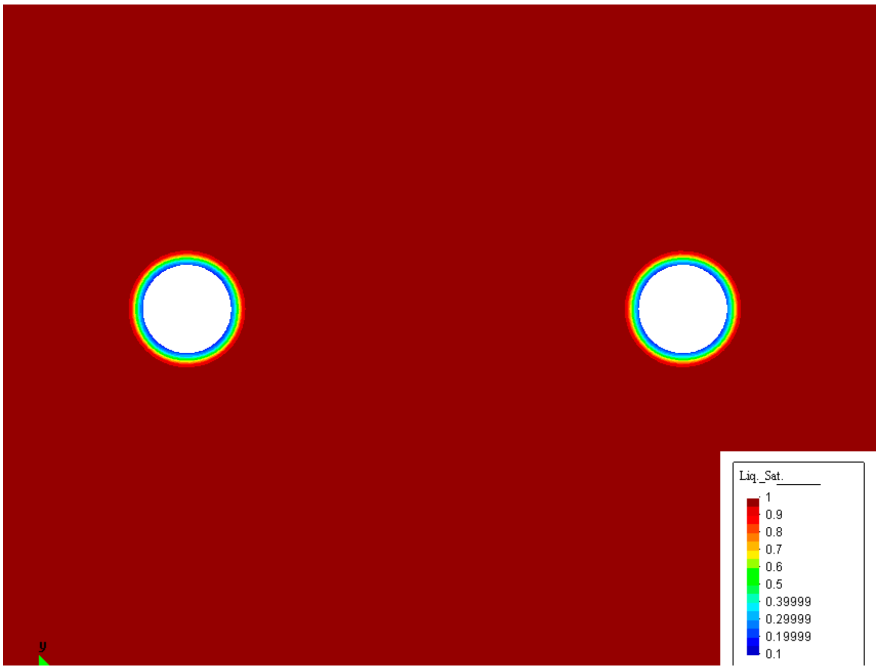

Figure 4-9. *Saturation degree contour after 33 days.*

4.2.5 References

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4.3 CODE "THAMES", M Chijimatsu HAZAMA (JNC), Y Sugita JNC

4.3.1 Description of numerical code THAMES of JNC

JNC has developed the coupled thermal, hydraulic and mechanical numerical analysis code THAMES, which can be used for describing processes in a saturated-unsaturated porous medium. The code has been validated by use of data from laboratory tests, engineered scale tests, and in-situ experiments.

4.3.2 Analysis objective

Analysis of the coupled thermal, hydraulic and mechanical process is carried out with the computer code named THAMES, which is a finite element code for analysis of coupled thermal, hydraulic and mechanical behaviors of a saturated-unsaturated medium. THAMES is extended to take account of the behavior in the buffer materials such as water flow due to thermal gradients, and swelling phenomena. The unknown variables are total pressure, displacement vector and temperature. The quadratic shape function is used for the displacements and linear one is used for total pressure and temperature.

4.3.3 Governing equations of coupled T-H-M process

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.

4.3.4 Assumptions

The governing equations 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 only in solid and liquid phases. The phase change of water from liquid to 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

4.3.5 Equilibrium equation

The equation of motion for a medium in a static case is known as an equilibrium equation. It is written in a total stress expression as:

$$\sigma_{ij,j} + \rho b_i = 0 \tag{24}$$

where σ_{ij} is the stress, ρ the density of as soil-water mixed medium and b_i the body force.

Terzaghi defined the effective stress principle and Bishop and Blight extended his definition and proposed the following equation for a saturated-unsaturated medium:

$$\sigma_{ij} = \sigma_{ij}^{'} + \chi \delta_{ij} \rho_f g \psi \tag{25}$$

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". Parameter χ is defined as:

$$\chi = 1 \quad \text{(Saturated zone)}, \quad \chi = \chi\,(S_r) \quad \text{(Unsaturated zone)} \tag{26}$$

χ is a nonlinear function of S_r (the degree of saturation).

At present it is assumed that χ is approximately equal to S_r.

Substituting equation (24) for equation (25), the equilibrium equation for the effective stress is a saturated-unsaturated geologic medium is obtained:

$$\left(\sigma_{ij}^{'} + \chi \delta_{ij} \rho_f g \psi\right)_{,j} + \rho b_i = 0 \tag{27}$$

where ($\chi \delta_{ij} \rho_f\, g \psi$) is a term which means that changes in the pressure head influence the equilibrium equation.

The effects of temperature can be implemented in a constitutive law for a sold medium. For an isotropic linear elastic material, Duhamel-Neuman's relationship can be used and the following constitutive law is obtained:

$$\sigma'_{ij} = C_{ijkl}\varepsilon_{kl} - \beta\delta_{ij}\left(T - T_o\right) \tag{28}$$

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.

The infinitesimal strain-deformation relationship is:

$$\varepsilon_{kl} = \frac{1}{2}\left(u_{k,l} + u_{l,k}\right) \tag{29}$$

where u_i is the deformation vector.

Substituting equation (25) and (26) into equation (24), the stress equilibrium equation is obtained. It takes into account the effects of temperature and pore pressure change:

$$\left|\frac{1}{2}C_{ijkl}\left(u_{k,l} + u_{l,k}\right) - \beta\delta_{ij}\left(T - T_o\right) + \chi\delta_{ij}\rho_f g\psi\right|_{,j} + \rho b_i = 0 \tag{30}$$

$(-\beta\delta_{ij}(T-T_o))_{,j}$ is a term which stands for the influence of heat transfer on the equilibrium equation.

4.3.6 Continuity equation for ground water

The equation of continuity for ground water in a saturated-unsaturated zone is derived from Richards' theory as follow:

$$\frac{\partial\left(\rho_f\theta\right)}{\partial t} = -\left(\rho_f v_i\right)_{,i} \tag{31}$$

where θ is the volumetric water content, t is the time and v_i is the velocity vector.

The equation of motion for ground water can be explained by Darcy's law. That is,

$$v_i = -k(\theta)_{ij} h_{,j} \tag{32}$$

where $k(\theta)_{ij}$ is the permeability tensor that is a function of θ. h is the total head.

The total head can be expressed as the sum of pressure head ψ and elevation head z:

$$h = \psi + z \tag{33}$$

The volumetric water content θ is a function of the degree of saturation S_r and porosity n, which is expressed as:

$$\theta = n\ S_r \tag{34}$$

Substitutions yield the following equation:

$$\left\{\rho_f\ k(\theta)_{ij}\ (\psi + z)_{,j}\right\}_{,i} = \frac{\partial}{\partial t}\rho_f\ n\ S_r \tag{35}$$

The right-hand side of equation (4-32) is expanded to:

$$\frac{\partial}{\partial t}\rho_f\ n\ S_r = n\ S_r\frac{\partial \rho_f}{\partial t} + \rho_f\ S_r\frac{\partial n}{\partial t} + \rho_f\ n\frac{\partial S_r}{\partial t} \tag{36}$$

The first term on the right-hand side represents density changes of the pore water. The second term means a change in the mineral skeleton of the porous medium. The third term stands for a change in degree of saturation in an unsaturated region.

Considering the compressibility and the thermal expansivity of water, the density of water can be expressed as:

$$\rho_f = \rho_{fo}\left[1 - \beta_T(T - T_o) + \beta_P(P - P_o)\right] \tag{37}$$

where P is the pore water pressure and ρ_{fo} is the reference density at $P=P_o$ and $T=T_o$.

β_T and β_P are the thermal expansivity and the compressibility of water, respectively,

$$\beta_T = \left|-\frac{1}{\rho_f}\frac{\partial \rho_f}{\partial T}\right| \quad (P = \text{constant}) \tag{38}$$

and

$$\beta_P = \left|\frac{1}{\rho_f}\frac{\partial \rho_f}{\partial P}\right| \quad (T = \text{constant}) \tag{39}$$

Eaton assumed that buoyancy could be ignored in an unsaturated zone due to its insignificant effect on the fluid flow. Adopting this assumption, β_T is set to be zero in an unsaturated zone. A combination of the first terms in equations (38) and (39) yields:

$$n\ S_r\frac{\partial \rho_f}{\partial t} = \rho_{fo}\ n\ S_r\ -\beta_T\frac{\partial T}{\partial t} + \beta_P\frac{\partial P}{\partial t} \tag{40}$$

The pressure head ψ is related to the pore water pressure as follows:

$$\psi = \frac{P}{\rho_f\, g} \tag{41}$$

Equation (41) can be modified to:

$$n\, S_r \frac{\partial \rho_f}{\partial t} = \rho_{fo}\, n\, S_r\ -\beta_T \frac{\partial T}{\partial t} + \rho_f\, g\, \beta_P \frac{\partial \psi}{\partial t} \tag{42}$$

Assuming that the strain is infinitesimal, the second and third terms on the right-hand side of equation (42) are expressed as:

$$\begin{aligned} &\rho_f\, S_r \frac{\partial n}{\partial t} \cong \rho_f\, S_r \frac{\partial u_{i,i}}{\partial t} \\ &\rho_f\, n \frac{\partial S_r}{\partial t} \cong \rho_f \frac{\partial (n\, S_r)}{\partial t} = \rho_f \frac{\partial \theta}{\partial t} = \rho_f \frac{\partial \theta}{\partial \psi} \frac{\partial \psi}{\partial t} \end{aligned} \tag{43}$$

Equation (43) is modified as follows:

$$\left\{\rho_f k(\theta)_{ij}\, h_{,j}\right\}_{,i} - \rho_{fo} n S_r \rho_f g \beta_P \frac{\partial \psi}{\partial t} - \rho_f \frac{\partial \theta}{\partial \psi} \frac{\partial \psi}{\partial t} - \rho_f S_r \frac{\partial u_{i,i}}{\partial t} + \rho_{fo} n S_r \beta_T \frac{\partial T}{\partial t} = 0 \tag{44}$$

Equation (44) is an equation of continuity for ground water which takes into account the compressibility of the ground water and changes in density by temperature changes.

4.3.7 Energy conservation law

In general, the ground consists of materials representing three phases, i.e., solids, liquids and gases. It is not easy to understand the behavior of heat transfer through such a composite material, because the way in which heat is transported is manyfold for each phase and heat transfer may occur between phases. Thus, the 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.

An energy conservation law, based upon the process proposed by Bear and Carapcioglu, is derived for ground water from the above assumptions without the effect of viscous dissipation.

Consideration the existence of an unsaturated zone, the equation of energy conservation is written as:

$$nS_r\rho_f C_{vf}\left(\frac{\partial T_f}{\partial t}+V_f\nabla T_f\right)=-\nabla nS_r J_f-\left(\frac{\partial P}{\partial T_f}\right)_{\rho_f} nS_r T_f\nabla V_f \tag{45}$$

where C_v is the specific heat and J is the heat flux by conduction. In equation (45), the first term at the left-hand side shows the time dependency of energy, the second term shows the change in energy due to heat convection. The first term at the right-hand side express the change in energy by heat conduction and the second term shows the reversible energy change caused by compression.

Similarly, the energy conservation law for a solid phase is written as:

$$(1-n)\rho_s C_{vs}\left(\frac{\partial T_s}{\partial t}+V_s\nabla T_s\right)=-\nabla(1-n)J_s-(1-n)\beta T_s\frac{\partial\varepsilon_s}{\partial t} \tag{46}$$

where subscript s means solid. In equation (46) the second term on the right-hand side indicates the reversible energy change caused by deformation.

Faust and Mercer proposed that the movement of water through porous media is so slow and the surface areas of all phases so large that it is reasonable to assume that a local thermal equilibrium among phase is achieved instantaneously. This means that the heat transfer between phases in the ground can be disregarded. If this assumption is permitted, the following equation is valid:

$$T=T_s=T_f \tag{47}$$

Using this assumption an equation of energy conservation for the ground can be defined:

$$\begin{aligned}&\left[nS_r\rho_f C_{vf}+(1-n)\rho_s C_{vs}\right]\frac{\partial T}{\partial t}+\left[nS_r\rho_f C_{vf}V_f+(1-n)\rho_s C_{vs}V_s\right]\nabla T\\&=\nabla\left[nS_r J_f+(1-n)J_s\right]-nS_r T\left(\frac{\partial P}{\partial T}\right)_{\rho_f}\nabla V_f-(1-n)T\beta\frac{\partial\varepsilon_s}{\partial t}\end{aligned} \tag{48}$$

Assuming that Fourier’s law is valid for heat conduction, the following equation apply:

$$\begin{aligned}J_f&=-K_{Tf}\nabla T\\J_s&=-K_{Ts}\nabla T\end{aligned} \tag{48}$$

where K_T is the coefficient of heat conduction.

The term $(\partial P / \partial T)$ in equation (33) can be modified as follows:

$$\frac{\partial P}{\partial T}_{\rho_f} = \left|\frac{\beta_T}{\beta_P}\right|_{\rho_f = \text{constant}} \tag{50}$$

Disregarding the velocity of a solid, equation (48) is rewritten in the following form:

$$\begin{aligned}&(\rho C_v)_m \frac{\partial T}{\partial t} + nS_r\rho_f C_{vf} V_{fi} T_{,i} - K_{Tm} T_{,ii} \\ &-nS_r T \frac{\beta_T}{\beta_P} k(\theta) h_{,ii} + \frac{1}{2}(1-n)\beta T \frac{\partial}{\partial t}\left(u_{i,j} + u_{j,i}\right) = 0\end{aligned} \tag{51}$$

where *(ρCv)m* and *KTm* are expressed as follows:

$$(\rho C_v)_m = nS_r\rho_f C_{vf} + (1-n)\rho_s C_{vs} \tag{52}$$

and

$$K_{Tm} = nS_r K_{Tf} + (1-n) K_{Ts} \tag{53}$$

Equation (53) is an energy conservation law in which the effects of stress-deformation and ground water flow are considered. The first, second and third terms on the right-hand side express changes in energy due to heat conduction, pore water pressure and reversible energy caused by solid deformation, respectively.

4.3.8 Governing equations

Equation (30), (44) and (51) represent the governing equations for a coupled thermal, hydraulic and mechanical problem proposed by Ohnishi et al. This model was verified with available analytical and experimental results. These equations are used with a total head expression such as:

$$\begin{aligned}&\left| \frac{1}{2} C_{ijkl}\left(u_{k,l} + u_{l,k}\right) - \beta\delta_{ij}\left(T - T_o\right) + \chi\delta_{ij}\rho_f g\psi \right|_{,j} + \overline{\rho_s} b_i = 0 \\ &\left\{\rho_f k(\theta)_{ij} h_{,j}\right\}_{,i} - \rho_{fo} nS_r \rho_f g\beta_P \frac{\partial h}{\partial t} - \rho_f \frac{\partial \theta}{\partial \psi}\frac{\partial h}{\partial t} - \rho_f S_r \frac{\partial u_{i,i}}{\partial t} + \rho_{fo} nS_r \beta_T \frac{\partial T}{\partial t} = 0 \\ &(\rho C_v)_m \frac{\partial T}{\partial t} + nS_r\rho_f C_{vf} V_{fi} T_{,i} - K_{Tm} T_{,ii} \\ &-nS_r T \frac{\beta_T}{\beta_P} k(\theta) h_{,ii} + \frac{1}{2}(1-n)\beta T \frac{\partial}{\partial t}\left(u_{i,j} + u_{j,i}\right) = 0\end{aligned} \tag{54}$$

where $\overline{\rho_s} = (1-n)\left(\rho_s - S_r\rho_f\right)$ and ρ_s is the density of a solid phase.

4.3.0 Governing equations of extended coupled T-H-M model for buffer material

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 is as follows:

$$\begin{aligned}&\xi\rho_l D_\theta \frac{\partial\theta}{\partial\psi}(h,_i - z,_i) + (1-\xi)\frac{\rho_l^2 gK}{\mu_l}h,_i \quad + \{\rho_l D_T T,_i\},_i \\ &-\rho_{lo} nS_r \rho_l g\beta_P \frac{\partial h}{\partial t} - \rho_l \frac{\partial\theta}{\partial\psi}\frac{\partial h}{\partial t} - \rho_l S_r \frac{\partial u_{i,i}}{\partial t} + \rho_{lo} nS_r \beta_T \frac{\partial T}{\partial t} = 0\end{aligned} \tag{55}$$

where D_θ is the isothermal water diffusivity, θ is the volumetric water content, ψ is the water potential head and K is the intrinsic permeability. The symbol ξ is the unsaturated parameter so that $\xi=0$ in the saturated zone, $\xi=1$ in the unsaturated zone. The symbol μ_l is the viscosity of water, ρ_l the density of water, and g the gravitational acceleration. D_T is the thermal water diffusivity, n the porosity, S_r the degree of saturation, β_P the compressibility of water, β_T the thermal expansion coefficient of water and z the elevation head. u_i is the displacement vector, T temperature, h the total head and t time. The subscript o means the reference state. This equation means that the water flow in the unsaturated zone is expressed by the diffusion equation and in the saturated zone by the Darcy's law.

The energy conservation equation has to treat the energy change by evaporation. The equation is given as:

$$\begin{aligned}&(\rho C_v)_m \frac{\partial T}{\partial t} + nS_r\rho_l C_{vl} V_{li} T,_i - K_{Tm} T,_{ii} + L \quad D_{\theta v}\frac{\partial\theta}{\partial\psi}(h,_i - z,_i) \quad ,_i \\ &+ nS_r T\frac{\beta_T}{\beta_P}\left\{\xi D_\theta \frac{\partial\theta}{\partial\psi}(h,_i - z,_i) + (1-\xi)\frac{\rho_l gK}{\mu_l}h,_i + D_T T,_i\right\},_i \\ &+ \frac{1}{2}(1-n)\beta T\frac{\partial}{\partial t}(u_{i,j} + u_{j,i})\delta_{ij} = 0\end{aligned} \tag{56}$$

where $(\rho C_v)_m$ is the specific heat of the material consisting of water and the soil particles, C_{vl} the specific heat of water, V_{li} the velocity vector of water, K_{Tm} the thermal conductivity of water and solid particles, L the latent heat of vaporization per unit volume and $D_{\theta v}$ the vapor diffusivity.

The equilibrium equation has to take the swelling behaviour into account.

$$\left[\frac{1}{2}C_{ijkl}(u_{k,l} + u_{l,k}) - F\pi\delta_{ij} - \beta\delta_{ij}(T - T_o) + \chi\delta_{ij}\rho_l g(h - z)\right] + \rho b_i = 0 \tag{57}$$

where C_{ijkl} is the elastic matrix, ρ the density of the medium and b_i the body force. χ is the parameter for the effective stress, $\chi=0$ in the unsaturated zone, $\chi=1$ in the saturated zone. The symbol F is the coefficient related to the swelling pressure process and $\beta = (3\lambda + 2\mu)\ \alpha_s$, where λ and μ are Lame's constants and α_s the thermal expansion coefficient.

The swelling pressure π can be assumed to be the function of water potential head (ψ) as follows:

$$\pi(\theta_1) = \rho_l g(\Delta\psi) = \rho_l g(\psi(\theta_1) - \psi(\theta_0)) = \rho_l g \int_{\theta_o}^{\theta_1} \frac{\partial\psi}{\partial\theta} d\theta \qquad (58)$$

where θ_0 is the volumetric water content in the initial state. This is compatible with the assumption that swelling pressure is equivalent to the water potential.

4.3.10 Initial and boundary conditions

It is necessary to establish the following initial and boundary conditions in order to solve the governing equations.

Initial conditions:

$$u_i(\tilde{x},t) = \hat{u}_i(\tilde{x},0) \qquad (59)$$

$$h(\tilde{x},t) = h(\tilde{x},0) \qquad (60)$$

$$T(\tilde{x},t) = T(\tilde{x},0) \qquad (61)$$

Boundary condition:

- Displacement; $u_i(\tilde{x},t) = \hat{u}_i(\tilde{x},t)$ (62)

  or traction; $\sigma_{ij}(\tilde{x},t)n_j(\tilde{x}) = \hat{T}_i(\tilde{x},t)$ (63)

- Total head; $h(\tilde{x},t) = \hat{h}(\tilde{x},t)$ (64)

  or flow rate; $\{k(\theta)h_{,i}\}n_i = -\hat{Q}(\tilde{x},t)$ (65)

- Temperature; $T(\tilde{x},t) = \hat{T}(\tilde{x},t)$ (66)

  or heat flow; $K_{Tm}T_{,i}n_i = -\hat{Q}_T(\tilde{x},t)$ (67)

where, $\tilde{x}$ is the position vector, n_j is the unit normal vector, $\hat{u}$ is the known displacement, $\hat{h}$ is the known head, $\hat{T}_i$ is the known surface traction, $\hat{Q}$ is the prescribed flow rate and $\hat{Q}_T$ is the prescribed heat flow.

4.3.11 Numerical techniques

The Galerkin type finite element technique is employed to formulate a finite element discretization. In order to obtain stable solutions, linear isoparametric elements are used to represent the behavior of total head h and temperature T. Quadratic isoparametric elements are used to express displacement u_i. In order to integrate time derivatives, a time weighting factor is introduced, and thus, any type of finite difference scheme may be applied.

4.4 CODE "ABAQUS", L. Börgesson, Clay Technology AB, Lund, Sweden (SKB)

4.4.1 General

The finite element code ABAQUS will be used for the calculations. ABAQUS is originally designed for non-linear stress analyses. It has been extended very much in the last 5-10 years and today has capability of describing a large range of processes in many different materials as well as complicated three-dimensional geometry.

The code includes special material models for rock and soil and ability to model geological formations with infinite boundaries and in situ stresses by e.g. the own weight of the medium. Detailed information of the available models, application of the code and the theoretical background is given in the ABAQUS Manuals.

The model of water-unsaturated swelling clay described in this chapter and used in these calculations is preliminary and especially the mechanical and vapour flux parts need to be improved.

4.4.2 Hydro-mechanical analyses in ABAQUS

The hydro-mechanical model consists of porous medium and wetting fluid and is based on equilibrium, constitutive equations, energy balance and mass conservation using the effective stress theory.

Equilibrium

Equilibrium is expressed by writing the principle of virtual work for the volume under consideration in its current configuration at time t:

$$\int_V \boldsymbol{\sigma} : \delta\boldsymbol{\varepsilon}\, dV = \int_S \mathbf{t} \cdot \delta\mathbf{v}\, dS + \int_V \hat{\mathbf{f}} \cdot \delta\mathbf{v}\, dV, \tag{68}$$

where $\delta\mathbf{v}$ is a virtual velocity field, $\delta\boldsymbol{\varepsilon} \overset{def}{=} sym(\partial\delta\mathbf{v}/\partial\mathbf{x})$ is the virtual rate of deformation, $\boldsymbol{\sigma}$ is the true (Cauchy) stress, $\mathbf{t}$ are the surface tractions per unit area, and $\hat{\mathbf{f}}$ are body forces per unit volume. For our system, $\hat{\mathbf{f}}$ will often include the weight of the wetting liquid:

$$\mathbf{f}_w = S_r n \rho_w \mathbf{g}, \tag{69}$$

where S_r is the degree of saturation, n the porosity, ρ_w the density of the wetting liquid and **g** is the gravitational acceleration, which we assume to be constant and in a constant direction (so that, for example, the formulation cannot be applied directly to a centrifuge experiment unless the model in the machine is small enough that g can be treated as constant). For simplicity we consider this loading explicitly so that any other gravitational term in $\hat{\mathbf{f}}$ is only associated with the weight of the dry porous medium. Thus, we write the virtual work equation as:

$$\int_V \boldsymbol{\sigma} : \delta\boldsymbol{\varepsilon} dV = \int_s \mathbf{t} \cdot \delta\mathbf{v} dS + \int_V \mathbf{f} \cdot \delta\mathbf{v} dV + \int_V S_r n \rho_w \mathbf{g} \cdot \delta\mathbf{v} dV, \tag{70}$$

where **f** are all body forces except the weight of the wetting liquid.

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

$$\overline{\boldsymbol{\sigma}}^* = \boldsymbol{\sigma} + \chi\, u_w \mathbf{I}. \tag{71}$$

where $\boldsymbol{\sigma}$ 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.

Energy balance

The conservation of energy implied by the first law of thermodynamics states that the time rate of change of kinetic energy and internal energy for a fixed body of material is equal to the sum of the rate of work done by the surface and body forces. This can be expressed as:

$$\frac{d}{dt} \int_V \left(\tfrac{1}{2} \rho \mathbf{v} \cdot \mathbf{v} + \rho U \right) dV = \int_s \mathbf{v} \cdot \mathbf{t} dS = \int_V \mathbf{f} \cdot \mathbf{v} dV, \tag{72}$$

where ρ is the current density,
v is the velocity field vector,
U is the internal energy per unit mass,
t is the surface traction vector,
f is the body force vector, and

Constitutive equations

The constitutive equation for the solid is expressed as:

$$d\boldsymbol{\tau}^c = \mathbf{H} : d\boldsymbol{\varepsilon} + \mathbf{g}, \tag{73}$$

where $d\boldsymbol{\tau}^c$ is the stress increment, **H** the material stiffness, $d\boldsymbol{\varepsilon}$ the strain increment and **g** is any strain independent contribution (e.g. thermal expansion). **H** and **g** are defined in terms of the current state, direction for straining, etc., and of the kinematic assumptions used to form the generalised strains.

The constitutive equation for the liquid (static) in the porous medium is expressed as:

$$\frac{\rho_w}{\rho_w^0} \approx 1 + \frac{u_w}{K_w} - \varepsilon_w^{th}, \tag{74}$$

where ρ_w is the density of the liquid, ρ_w^0 is its density in the reference configuration, $K_w(T)$ is the liquid's bulk modulus, and

$$\varepsilon_w^{th} = 3\alpha_w(T - T_w^0) - 3\alpha_{w|T^I}(T^I - T_w^0) \tag{75}$$

is the volumetric expansion of the liquid caused by temperature change. Here $\alpha_w(T)$ is the liquid's thermal expansion coefficient, T is the current temperature, T^I is the initial temperature at this point in the medium, and T_w^0 is the reference temperature for the thermal expansion. Both u_w/K_w and ε_w^{th} are assumed to be small.

Mass conservation

The mass continuity equation for the fluid combined with the divergence theorem implies the pointwise equation:

$$\frac{1}{J}\frac{d}{dt}(J\rho_w S_r n) + \frac{\partial}{\partial \mathbf{x}} \cdot (\rho_w S_r n \mathbf{v}_w) = 0. \tag{76}$$

where J is the determinant of the Jacobian matrix and **x** is position. The constitutive behaviour for pore fluid is governed by Darcy's law, which is generally applicable to low fluid velocities. Darcy's law states that, under uniform conditions, the volumetric flow rate of the wetting liquid through a unit area of the medium, $S_r n \mathbf{v}_w$, is proportional to the negative of the gradient of the piezometric head:

$$S_r n \mathbf{v}_w = -\hat{\mathbf{k}}\frac{\partial \phi}{\partial \mathbf{x},} \tag{77}$$

where $\hat{\mathbf{k}}$ is the permeability of the medium and ϕ is the piezometric head, defined as:

$$\phi \overset{\text{def}}{=} z + \frac{u_w}{g\rho_w} \tag{78}$$

where z is the elevation above some datum and g is the magnitude of the gravitational acceleration, which acts in the direction opposite to z. $\hat{\mathbf{k}}$ can be anisotropic and is a function of the saturation and void ratio of the material. $\hat{\mathbf{k}}$ has units of velocity (length/time). [Some authors refer to $\hat{\mathbf{k}}$ as the hydraulic conductivity and define the permeability as:

$$\hat{\mathbf{K}} = \frac{\nu}{g}\hat{\mathbf{k}} \tag{79}$$

where ν is the kinematic viscosity of the fluid.]

We assume that g is constant in magnitude and direction, so:

$$\frac{\partial \phi}{\partial \mathbf{x}} = \frac{1}{g\rho_w}\left(\frac{\partial u_w}{\partial \mathbf{x}} - \rho_w \mathbf{g}\right) \tag{80}$$

Vapour flow

Vapour flow is modelled as a diffusion process driven by a temperature gradient (coded as UEL user supplied routine with stiffness and flow).

$$\mathbf{q}_v = -D_{Tv} \frac{\partial T}{\partial \mathbf{x}} \tag{81}$$

where $\mathbf{q}_v$ is the vapour flux and D_{Tv} the thermal vapour diffusivity.

4.4.3 Uncoupled heat transfer analysis

Energy balance

The basic energy balance is:

$$\int_v \rho \dot{U} dV = \int_s q dS + \int_v r dV \tag{82}$$

where V is a volume of solid material, with surface area S; ρ is the density of the material; $\dot{U}$ is the material time rate of the internal energy; q is the heat flux per unit area of the body, flowing into the body; and r is the heat supplied externally into the body per unit volume.

It is assumed that the thermal and mechanical problems are uncoupled in the sense that $U = U(T)$ only, where T is the temperature of the material, and q and r do not depend on the strains or displacements of the body. For simplicity a Lagrangian description is assumed, so ”volume” and ”surface” mean the volume and surface in the reference configuration.

Constitutive definition

The relationship is usually written in terms of a specific heat, neglecting coupling between mechanical and thermal problems:

$$c(T) = \frac{dU}{dT}, \tag{83}$$

Heat conduction is assumed to be governed by the Fourier law:

$$\mathbf{f} = -\mathbf{k} \frac{\partial T}{\partial \mathbf{x}} \tag{84}$$

where $\mathbf{f}$ is the heat flux and $\mathbf{k}$ is the heat conductivity matrix, $\mathbf{k} = \mathbf{k}(T)$. The conductivity can be fully anisotropic, orthotropic, or isotropic.

4.4.4 Coupling of thermal and hydro-mechanical solutions

In ABAQUS the coupled problem is solved through a ”staggered solution technique” as sketched in Figure 4-10 and below:

1. First a thermal analysis is performed where heat conductivity and specific heat are defined as functions of saturation and water content. In the first analysis these parameters are assumed to be constant and in the subsequent analyses they are read from an external file.

2. The hydromechanical model calculates stresses, pore pressures, void ratios, degree of saturation etc. as function of time. Saturation and void ratio histories are written onto an external file.

3. The material parameters update module reads the file with saturation and void ratio data and creates a new file containing histories for saturation and water content. The saturation and water content histories are used by the thermal model in the following analysis.

4. Steps 1-3 are repeated if parameter values are found to be different compared to those of the previous solution.

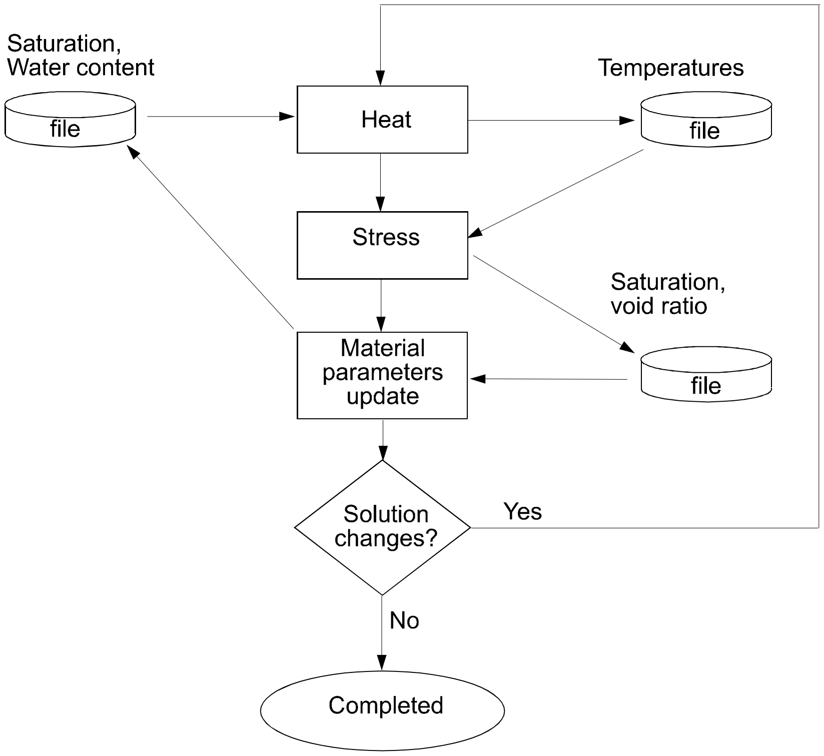

Figure 4-10*. In ABAQUS, heat transfer calculations and hydro-mechanical calculations are decoupled. By using the iteration procedure schematically shown above, the effects of a fully coupled THM model are achieved.*

4.4.5 Description of the parameters of the material model of the buffer

Processes

Thermal flux from conduction

The only thermal flux that is modelled is thermal conduction using the following parameters:

λ = thermal conductivity
c = specific heat

Water liquid flux

The water flux in the liquid phase is modelled to be governed 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 according to Eq (85):

$$\boldsymbol{K_p} = (\boldsymbol{S_r})^{\delta} \boldsymbol{K} \tag{85}$$

where

$\boldsymbol{K_p}$ = hydraulic conductivity of partly saturated soil (m/s)
$\boldsymbol{K}$ = hydraulic conductivity of completely saturated soil (m/s)
δ = parameter (usually between 3 and 10)

Water transport driven by gravity and density gradients is included in the model as well.

Water vapour flux

The water vapour flux is modelled as a diffusion processes driven by the temperature gradient and the water vapour pressure gradient (at isothermal conditions) according to Eq (86):

$$q_v = -D_{Tv}\nabla T - D_{pv}\nabla p_v \tag{86}$$

where
$\boldsymbol{q_v}$ = vapour flow
$\boldsymbol{D_{Tv}}$ = thermal vapour flow diffusivity
$\boldsymbol{T}$ = temperature
$\boldsymbol{D_{pv}}$ = isothermal vapour flow diffusivity
$\boldsymbol{p_v}$ = vapour pressure

The isothermal vapour flow is neglected and thus D_{pv} =0. The thermal water vapour diffusivity D_{Tv} can be evaluated from moisture redistribution tests by calibration calculations. The following relations were found to yield acceptable results:

$$\boldsymbol{D_{Tv} = D_{Tvb}} \qquad 0.3 \le S_r \le 0.7 \tag{87}$$

$$D_{Tv} = D_{Tvb} \cdot cos^{a}\left| \frac{S_r - 0.7}{0.3} \cdot \frac{\pi}{2} \right| \qquad S_r \ge 0.7 \tag{88}$$

$$D_{Tv} = D_{Tvb} \cdot sin^{b}\left| \frac{S_r}{0.3} \cdot \frac{\pi}{2} \right| \qquad S_r \le 0.3 \tag{89}$$

where

a and *b* are factors that regulates the decreased vapour flux at high and low degree of saturation.

The diffusivity is thus constant with a basic value D_{Tvb} between 30% and 70% degree of saturation. It decreases strongly to D_{Tv}=0 at 0% and 100% saturation. The influence of temperature and void ratio on the diffusivity is not known and not considered in the model.

4.4.6 Hydraulic coupling between the pore water and the pore gas

The pore pressure u_w of the unsaturated buffer material, which is always negative, is modelled as being a function of the degree of saturation S_r independent of the void ratio.

$$u_w = f(S_r) \tag{90}$$

ABAQUS also allows for hysteresis effects, which means that two curves may be given (drying and wetting curves). The pore air pressure is not modelled.

4.4.7 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 represented by Eqs 87-90. The shortcoming of the effective stress theory is compensated for by a correction called moisture swelling.

The *Porous Elastic Model* implies a logarithmic relation between the void ratio *e* and the average effective stress *p* according to Eq (91).

$$\Delta e = \kappa \Delta \ln p \tag{91}$$

where κ = porous bulk modulus
Poisson's ratio ν is also required.

The *Drucker Prager Plasticity* model contains the following parameters:

β = Friction angle in the *p*-*q* plane
d = Cohesion in the *p*-*q* plane
ψ = Dilation angle
q = $f(\varepsilon^d_{pl})$ = yield function

The yield function is the relation between Mises' stress q and the plastic deviatoric strain ε^d_p for a specified stress path. The dilation angle determines the volume change during shear.

4.4.8 Thermal expansion

The volume change caused by the thermal expansion of water and particles can be modelled with the parameters:

α_s = coefficient of thermal expansion of solids (assumed to be 0)
α_w = coefficient of thermal expansion of water

Only the expansion of the separate phases is taken into account. The possible change in volume of the structure 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.

4.4.9 Mechanical behaviour of the separate phases

The water and the particles are mechanically modelled as separate phases with linear elastic behaviour. The pore air is not mechanically modelled.

4.4.10 Mechanical coupling between the microstructure and the pore water

Effective stress theory

The effective stress concept according to Bishop is used for modelling the mechanical behaviour of the water-unsaturated buffer material:

$$s_e = (s - u_a) + \chi(u_a - u_w) \tag{92}$$

Eq (92) is simplified in the following way:

$u_a = 0$ (no account is taken to the pressure of enclosed air)
$\chi = S_r$

Moisture swelling

The shortcomings of the effective stress theory can be partly compensated in ABAQUS by a correction called ”moisture swelling”. This procedure changes the volumetric strain ε_v by adding a strain that can be made a function of the degree of saturation S_r:

$$\Delta\varepsilon_v = f(S_r) \tag{93}$$

4.4.11 Required parameters

The required input parameters for the described THM model (ABAQUS) are the following:

Thermal

- Tables of thermal conductivity λ and specific heat c as function of void ratio e and degree of saturation S_r.

Hydraulic

- Table of the hydraulic conductivity of water saturated material K as function of void ratio e and temperature T.
- Influence of degree of saturation S_r on the hydraulic conductivity K_p expressed as the factor δ in Eq (68).
- The basic water vapour flow diffusivity D_{vTb} and the parameters a and b in Eqs 70 to 72.
- Table of the matric suction u_w as a function of the degree of saturation S_r.

Mechanical

- Porous bulk modulus κ according to Eq (74) and Poisson’s ratio ν.
- Drucker Prager plasticity parameters β, d, ψ, and the yield function.
- Bulk modulus and coefficient of thermal expansion of water (B_w, α_w)and bulk modulus solids (B_s).
- Bishops parameter χ in Eqn 75 (usual assumption $\chi = S_r$).
- The volume change correction ε_v as a function of the degree of saturation S_r (the ”moisture swelling” procedure).

- *Initial conditions*

The following initial conditions of the elements in the structure need to be specified:
- void ratio e
- degree of saturation S_r
- pore pressure u
- average effective stress p

4.5 CODE “ROCKMECH”, "Fully Coupled T -H-M Model", L. Liedtke (BGR)

4.5.1 Introduction

Problems of practical interest to underground activities include water supply, exploitation of petroleum reservoirs, utilization of geothermal energy (hydrothermal or hot dry rock reservoirs), safe deposition of waste (repositories for domestic,toxic, and radioactive waste), and geotechnical applications (construction of tunnels, caverns, stability analyses of structures and buildings). A major task of the theoretical hydrogeology is, therefore, to describe the fundamental processes of flow, transport, and deformation of soil and rock, and to develop models with predictive competence.

The general present task is to investigate the coupled thermo-hydro-mechanical behavior of composite waste-buffer-rock systems placed in deep excavations.

4.5.2 Basics

The following principles are basic to the model:

- Effective stress and consolidation concepts (Biot 1941, Terzaghi 1943).
- 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 the stress deviators (1952).
- Roscoe/Schofield/Burland's (1958-1971) Cam-Clay-Model.

Realistic THM modelling requires 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. For the buffer one 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 a major role.
- Formation and transport of vapour.
- Osmosis.

4.5.3 Hydrothermal effects

The most important hydrothermal effects caused by thermal and pressure gradients 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).

4.5.4 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.

4.5.5 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.

4.5.6 Barrier zonation

It is useful to define zones of particular importance in the modelling. Such zones may be the buffer and the backfill as well as the EDX and near-field and far-field rock. They are all affected in different ways by temperature and temperature gradients, water transport and gas migration. A particularly important issue is the structure of the near-field rock since it determines the rate with which the buffer is supplied with water and also where rock water will be available for water uptake by the buffer clay.

4.5.7 Basic equations

Balance

- We consider flow of two fluid phases (compressible and incompressible fluids) in a deformable thermo-poro-elastic porous medium based on Biot's consolidation concept. No phase change of water beyond 100°C are considered.

- There are four unknown field functions to determine: gas pressure p_g, water pressure p_W, solid displacements, *u,* and equilibrium temperature *T*.

- The followings steps are conducted to derive the governing equations:

- applying the constitutive relationships to the balance equations,
- combining mass and momentum balance equations for fluid flow,
- introducing physically based simplifications.

The general theory of porous media formating the basis of the selected governing equations is found in Bear & Bachmat (1990), Lewis & Schrefler (1998), de Boer (2000), and Kolditz (2000).

Components

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 (Gawin et al. 1995).

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.

4.5.8 Example of numerical calculation using the model

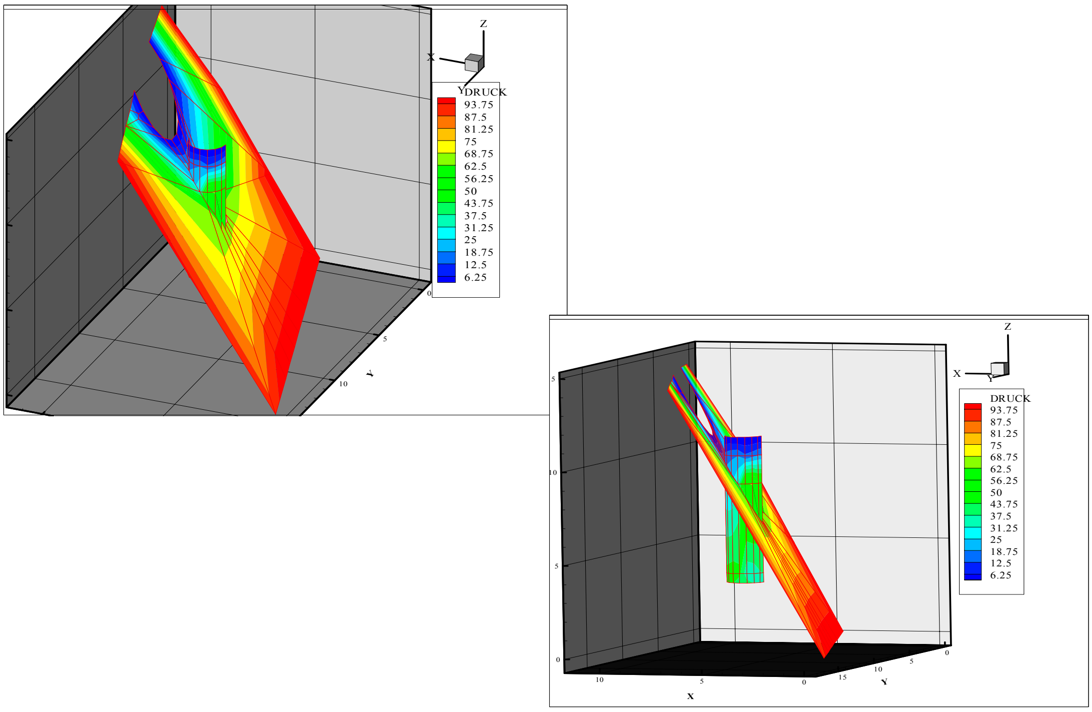

Figure 4-11. *Example of result of numerical calculation of the hydraulic heads in the buffer clay and a dipping fracture that intersects the hole and buffer.*

6. CHEMICAL MODELLING , CODE “PHREEQ-C2 and NETPATH”, A.Lukkonen, VTT (POSIVA)

6.1 Objectives

The Prototype repository project conducts an integrated full-scale repository test of the KBS-3 system. The test comprises the technical (deposition of canisters, backfilling, instrumentation of the backfill and the repository surroundings, etc.), the monitoring (repetitive recording of thermo/hydro/mechanical data, and water/gas samplings) and the modelling (conceptual/mathematical modelling of the repository) parts.

The Posiva/VTT co-operation in the project aim to concentrate to modelling of groundwater chemistry at the interface of the backfill and the near-field rock. The time-series sampling of groundwater gives several possibilities to study and evaluate the groundwater chemical processes occurring during the Prototype test. There are several points of interest. Within the Fifth Framework programme, however, the aim is to study chemical changes mostly at the repository surroundings as a function of time. There are several geochemical aspects related to the bentonite performance within the repository but currently these studies have to be ruled out because of the timetable problems explained below.

According to the timetable given, all geochemical modelling will mostly concentrate on the data collected from the near-field double packer sections before the backfilling of the repository (e.g. Andersson & Säfvestad 2000). The time-span between the activation of Section I and the delivery of predictive modelling results is only a couple months. This practically rules out the utilisation of the time-series data from the backfill sampling vessels in the predictive modelling. However, the comparisons between the predictive modelling and measured data should be finished by summer 2003. This makes possible to use the vessel samplings at least as a reference material.

6.2 Model concept and formulation

The modelling task is divided into two parts. The analysed water samples from the near-field rock (March ‘98 -> spring ’02) around the Sections I & II 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. The inverse modelling is done with 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. (2000a) have specified certain properties of the VOLCLAY bentonite. Similarly, Huertas et al. (2000b) have recently reported the effects of heat up of a repository in the FEBEX project. The beginning of year 2002 may produce some initial results from the operating Prototype repository and this data could be used as support or reference for predictions.

The forward modelling software will be PHREEQC-2. The predictions can be done either as batch mixing/reaction studies or as 1D mixing/reaction path studies. In the case of batch mixing/reaction studies the predictions concentrate to 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 (Ball & Nordstrom 1991), EQ3/6 compatible LLNL.DAT (based on ”thermo.com.V8.R6.230” by Jim Johnson, LLNL) and NAGPSI_1.DAT (Pearson & Waber 1999).

The predictions will be reported in spring 2002, and they extend at least one year forward. The comparisons between the measured data and predictions are reported by the spring 2003. The complete Fifth Framework programme final report shall be delivered by the beginning of 2004.

6.3 Expected outcome

Current studies within the Fifth Framework programme emphasise the initial conditions of the Prototype repository. The chemical data used in the studies consist a time-series that is mostly or only before the date of the repository activation. It is possible, however, that the heat up effects on hydraulic flow field and chemical reaction rates. Furthermore, the backfill bentonite may affect the chemical composition and colloid content of the near-field groundwater. Within the Framework programme timetable, the effects of the operational repository must be estimated with a priori knowledge from elsewhere.

However, the definition of the initial geochemical conditions establishes a solid basis for the further studies of the operational repository. Moreover, the blind prediction exercise of the effects of the operational repository tests 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.

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8. COMMENTS

The present document is meant to be a presentation of the conceptual model and the various numerical codes for describing the evolution and performance of the buffer clay of the KBS3 concept. No attempt has been made here to assess the models or to find out how they agree mutually or with the real processes on site, which is a matter for forthcoming work.

For the sake of simplicity and for making unanimous reference to the mathematical expressions representing the different codes possible the equations have been numbered currently in succession.

9. ACKNOWLEDGEMENTS

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