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Report on THM/THMC model improvement

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Summary

This report corresponds to Deliverable 10 of the THERESA project, financed by EC 6th FP Euratom in the field of radioactive waste management, and it concerns the work performed within Work Package 4 (WP4). The objective of this Deliverable is twofold. On the one hand, the state of the formulations and constitutive laws at the start of the project (January 2007) of the six computer codes participating in WP4 are described. They correspond to the six different teams contributing to the WP. On the other hand, the code and constitutive model improvements proposed by the six teams are described.

Considering the set of codes, there is a large area of common ground between them but differences in detail, scope and approaches have been identified. Generally, the formulations adopted place the codes in a good position for a successful modelling of the coupled THM processes in the buffer. THMC analyses are in principle feasible for four of the codes. In spite of the quite powerful existing formulations in all the codes, an impressive range of proposed improvements has been put forward by the various teams.



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1. Introduction

Within the THERESA project, Work Package 4 (WP4) is concerned with the development of constitutive and numerical modelling capabilities to simulate coupled THM and/or THMC processes in buffer and rock-buffer interfaces, with regards to their effects on the performance and safety of underground waste repositories.

Under this overall objective, the focus of research is placed on:

- Extension of existing constitutive models (and computer codes) of buffer materials and rock-buffer or canister-buffer interfaces for coupled THM and/or THMC processes
- Benchmark Tests (BMT) for validation of the enhanced constitutive models and computer codes.
- Applications of the developed models and codes to the simulation of an existing large scale test case.

The present Deliverable refers to the first of the points above and contains a summary description of the formulations underlying the various codes as well as the areas that have been identified for further improvements and developments. The codes included in WP4 and the teams responsible for them are listed in Table 1. The information included in the Deliverable is based on the individual reports submitted by the modelling teams: CIMNE (Zandarín et al., 2008), Marintel (Lempinen 2008), KTH (Tong & Jing, 2008), Quintessa (Maul & Benbow, 2006, Bond et al., 2008, Bond & Watson, 2008), Cardiff University, CU (Thomas et al., 2008) and IRSN (Millard 2008). Initially, IRSN proposed the use of the VIPLEF code (Tijani 2007), but it was later replaced by the CAST3M code.

The Deliverable concludes with a summary of the formulations and perceived capabilities of the codes examined. The WP4 output is an input to WP5 where a Technical Audit (TA) is performed on the work carried out in WP4 involving the numerical modelling capabilities for processes occurring in the buffer and in the buffer-rock interfaces, with consideration of coupled processes, as related to the assessment of the performance and safety of underground nuclear waste repositories. Consequently, the present Deliverable has a descriptive character, evaluation being the objective of WP5.

Table 1. Codes and teams in WP4

CODE	TEAM
Code-Bright	CIMNE
FreeFEM++	Marintel
ROLG	KTH
QPAC-EBS	Quintessa
COMPASS	CU
CAST3M	IRSN



2. Description of computer codes.

In this section, the computer codes used in WP4 are summarily described, based on the information provided in the reports contributed by the teams responsible. Special attention is given to the basic mathematical formulation and the constitutive laws used, as they relate to the processes that are taken into consideration. The description of the code includes:

- General code information: processes concerned, dimensionality, numerical methods (such as FEM or FDM), and special features important to WP4
- Equation for mechanical behaviour: equations of motion and constitutive models;
- Equations for hydraulic behaviour;
- Equations for thermal behaviour;
- Equations for transport processes;
- Equations for geochemical processes;

Not every aspect is included in all codes, as indicated in the final summary below.

2.1. CIMNE (CODE_BRIGHT)

Code_Bright is a Finite Element Programme that allows the solution of coupled and uncoupled thermo-hydro-mechanical problems. The types of analysis can be 1D (uni-axial confined strain and axisymmetric), 2D (plane strain and axisymmetric) and fully 3D.

The constitutive laws are defined by a set of parameters with alternative types of relations for different application cases.

The types of boundary conditions are:

- 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.

The convergence criteria are defined by tolerances for absolute and relative error independent for each unknown, and tolerance for residual convergence of each problem (mechanical, hydraulic, etc.). The output options include spatial distribution of variables at user defined time points, and time evolution of variables at user-defined space points.



2.1.1. Mathematical formulation.

The code solves simultaneously the fundamental balance equations:

- Mass balance of water:

$$\frac{\partial}{\partial t}(\omega_l \rho_l S_l \phi + \omega_g^w \rho_g S_g \phi) + \nabla \cdot (\mathbf{j}_l^w + \mathbf{j}_g^w) = f^w \quad (2.1.1)$$

- Mass balance of air:

$$\frac{\partial}{\partial t}(\omega_l^a \rho_l S_l \phi + \omega_g^a \rho_g S_g \phi) + \nabla \cdot (\mathbf{j}_l^a + \mathbf{j}_g^a) = f^a \quad (2.1.2)$$

- Internal energy balance for the medium:

$$\frac{\partial}{\partial t}(E_s \rho_s (1 - \phi) + E_l \rho_l S_l \phi + E_g \rho_g S_g \phi) + \nabla \cdot (\mathbf{i}_c + \mathbf{j}_{Es} + \mathbf{j}_{El} + \mathbf{j}_{Eg}) = f^Q \quad (2.1.3)$$

- Momentum balance of the medium:

$$\nabla \cdot \boldsymbol{\sigma} + \mathbf{b} = \mathbf{0} \quad (2.1.4)$$

where:

ϕ : porosity	\mathbf{b} : body forces,
ρ : density	ω : mass fraction,
\mathbf{j} : total mass flux	$\omega\rho$: mass content per unit volume of phase,
\mathbf{i} : non-advective mass flux	E : specific internal energy
\mathbf{q} : advective flux	\mathbf{i}_c : conductive heat flux
\mathbf{u} : solid displacements	\mathbf{j}_E : energy fluxes due to mass motion
$\boldsymbol{\sigma}$: stress tensor	
S_l, S_g : degree of saturation of liquid and gas phases i.e., fraction of pore volume occupied by each phase.	
Superscripts w and a refer to water and air, respectively	
Subscripts s, l and g refer to solid, liquid and gas phase, respectively.	
(Note: Bold non italic symbols denote vector or tensor)	



2.1.2. Mechanical constitutive law.

The mechanical constitutive law is based on the Basic Barcelona Model (assuming a viscoplastic formulation for numerical implementation), and linear elasticity behaviour is assumed for other materials.

The strain terms are defined as:

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^e + \boldsymbol{\varepsilon}^{VP}; \quad \boldsymbol{\varepsilon}^e = \boldsymbol{\varepsilon}^{stress} + \boldsymbol{\varepsilon}^{thermal} + \boldsymbol{\varepsilon}^{suction}; \quad \boldsymbol{\varepsilon}^{stress} = \mathbf{D}^{-1} \boldsymbol{\sigma} \quad (2.1.5)$$

$$\boldsymbol{\varepsilon}^{VP} = \left[\Gamma \langle \phi(F) \rangle \frac{\partial G}{\partial \boldsymbol{\sigma}} \right] \text{ (Perzyna model)} \quad (2.1.6)$$

where $\boldsymbol{\varepsilon}^e$ is the elastic strain tensor (with stress, temperature and suction terms), \mathbf{D} is the elasticity tensor, $\boldsymbol{\varepsilon}^{VP}$ the viscoplastic strain rate tensor, Γ is the viscoplastic parameter, $\langle \phi(F) \rangle$ is the plastic flow function, F is the yield surface, G is the plastic potential function, $\langle \phi(F) \rangle = (F/F_0)^N$, where F_0 is a reference stress, N is a parameter of the model, and the Makulay brackets are used.

The model uses the effective stress and suction as state variables. Effectives stress is defines as $\sigma' = \sigma - \max(P_g, P_l)$.

The thermal expansion of materials is considered. The parameters of the constitutive laws change with temperature and suction. The elastic terms in equation (2.15) related to temperature and suction are obtained from the following equation for volumetric deformations: $\Delta \varepsilon_v = 3b_s \Delta T + 3a_s \Delta (P_g - P_l)$ where a_s (MPa⁻¹) is swelling coefficient for changes in suction and b_s (°C⁻¹) is a linear thermal expansion coefficient for the medium.

Integration of (2.1.5) gives the stress increments as a function of the strain increments, temperature increments and suction increments. The triaxial yield surface and plastic potential functions to be used in (2.1.5) are:

$$F(p, q, s) = q^2 - M^2 [p + p_s(s)] [p_o(s) - p] = 0 \quad (2.1.7)$$

$$G(p, q, s) = q^2 - \alpha M^2 [p + p_s(s)] [p_o(s) - p] = 0 \quad (2.1.8)$$

where p is the net average stress, q is the deviatoric stress, s is the matrix suction, M is the slope of critical state shear strength, α is the parameter that defines the non-associative of plastic potential (with $\alpha = 1.0$ indicating an associate flow rule),

$p_s(s) = k_s s$, and k_s the material parameter that controls the increase in cohesion with suction, respectively. Parameter P_0 represents the loading-collapse curve (LC), is given by

$$p_o(s) = p^c \left(\frac{p_o^*}{p^c} \right)^{\frac{\lambda(0)-\kappa}{\lambda(s)-\kappa}} \quad (2.1.9)$$

where p^c is the reference stress of the loading-collapse curve, p_o^* is the initial yield mean net stress, and $\lambda(0) - \kappa$ is the virgin compressibility for saturated condition, with $\lambda(0)$ being the slope of the virgin elastic compressibility for saturated condition and κ the slope of the unload-reload line. The parameter $\lambda(s)$ is the volumetric compressibility index, written as

$$\lambda(s) = \lambda(0) [(1-r)\exp(-\beta s) + r] \quad (2.1.10)$$

where r is the parameter that establishes the minimum value of the compressibility index for high values of suction, and β is the parameter that controls the rate of increase in stiffness with suction.

The hardening law is given as

$$dp_o^* = \frac{(1+e)p_o^*}{\lambda(0) - \kappa} d\varepsilon_v^p \quad (2.1.11)$$

where e is the void ratio, and $d\varepsilon_v^p$ is the plastic volumetric strain increment.

The stress-strain constitutive law is a thermo-elasto-plastic model for unsaturated soils.

The thermal expansion of materials is considered. The parameters of the constitutive laws change with temperature and suction.

2.1.3. Hydraulic constitutive law.

Liquid and air advective fluxes

Advection of water and air in gas and liquid phases is calculated by means Darcy's law.

$$\mathbf{q}_\alpha = -\frac{\mathbf{k}k_{r\alpha}}{\mu_\alpha} (\nabla P_\alpha - \rho_\alpha \mathbf{g}) \quad (2.1.12)$$



with the permeability tensor defined by

$$\mathbf{k} = \mathbf{k}_o \frac{\phi^3}{(1-\phi)^2} \frac{(1-\phi_o)^2}{\phi_o^3} \quad (2.1.13)$$

where : \mathbf{q}_α : is the flow rate in the porous media, \mathbf{k} : is the intrinsic permeability for the matrix at porosity ϕ , \mathbf{k}_o : is the intrinsic permeability for the matrix at porosity ϕ_o , $k_{r\alpha}$: is the phase relative permeability of phase α , μ_α : is the viscosity of the fluid phase α , P_α : is the pressure of the fluid phase α , ρ_α : the density of the fluid phase α , \mathbf{g} : is the vector of gravitational acceleration.

The fluid density changes with temperature and with pressure. The intrinsic permeability changes with porosity. The hydraulic conductivity is affected by fluid viscosity, which changes with temperature. The density of water is calculated as $\rho_\alpha = \rho_{\alpha 0} \exp(\beta(P_l - P_{l0}) + \alpha(T - T_0))$ where β is the fluid compressibility and α is a volumetric expansion coefficient.

The viscosity is calculated as $\mu_l = A \exp(B/(273.15 + T))$ with $A = 2.1 \times 10^{-2}$ (MPa) and $B = 1808.5$ (K⁻¹). For the gas phase, the ideal gases law is used.

Relative permeability is considered with the van Genuchten function or a power of degree of saturation: $k_{r\alpha} = \sqrt{S_l} \left(1 - (1 - S_l^{1/\lambda})^\lambda\right)^2$; $k_{r\alpha} = (S_l)^n$.

A coupling of flow and deformations is achieved via Kozeny equation (2.1.13) and the thermal coupling is achieved considered the changes of fluid properties with temperature. However, primary couplings arise from balance equations.

Retention curve

The hydraulic conductivity of the materials considered depends on their degree of saturation. The retention curve (Van Genuchten Model) is

$$S_e = \frac{S_l - S_{rl}}{S_{ls} - S_{rl}} = \left[1 + \left(\frac{P_g - P_l}{P} \right)^{1/(1-\lambda)} \right]^{-\lambda} \quad (2.1.14)$$

$$P = P_o \frac{\sigma}{\sigma_o} \quad (2.1.15)$$

The dependence of the surface tension with temperature is calculated using:

$$\sigma_0(T) = 0.03059 \exp\left(\frac{252.93}{273.15 + T}\right) \quad (2.1.16)$$

where: S_e : is the degree of saturation of porous media, S_l : is the degree of saturation of liquid, S_{rl} : is the residual degree of saturation, S_{ls} : is the maximum degree of saturation λ : is the shape function coefficient for the retention curve, P_o : is the pressure of air entrance at a reference temperature, σ_o is the surface tension at a temperature at which P_o was measured, σ : is the surface tension at temperature T .

Non-advective fluxes. Molecular diffusion

The molecular diffusion is governed by Fick's law

$$\mathbf{i}_\alpha^i = -(\phi \rho_\alpha S_\alpha D_\alpha^i \mathbf{I}) \nabla \omega_\alpha^i \quad (2.1.17)$$

where \mathbf{i}_α^i is the non-advective mass flux vector⁽ⁱ⁾, ϕ the porosity of porous media, ρ_α is the density of the phase α , S_α is the degree of saturation of the phase α , D_α^i is the diffusion coefficient⁽ⁱ⁾, and ω_α^i is the mass fraction⁽ⁱ⁾. The superindex i refers to species, and the subindex α refers to phases. \mathbf{I} is the identity tensor.

The diffusion coefficient of vapour is given by:

$$D_\alpha^{vapor} = \tau D^v \left(\frac{(273.15 + T)^n}{P_g} \right) \quad (2.1.18)$$

where τ is the tortuosity and D^v is the coefficient of diffusion, where $D = 5.9 \times 10^{-6} \text{ m}^2/\text{s}/\text{K}^{-n}\text{Pa}$. The default value for n is 2.3.

The diffusion coefficients of dissolved salt and air are given by

$$D_\alpha^{air \text{ or } solute} = \tau D \exp\left(\frac{-Q}{R(273.15 + T)}\right) \quad (2.1.19)$$

where Q the molar heat capacity and R is the ideal gas constant, where $D = 1.1 \times 10^{-4}$ m²/s and $Q = 24530$ J/mol.

Mass fractions and densities of the gas phase are calculated using the ideal gas law. Vapour pressure as a function of temperature and suction is obtained as

$$P_v(T, P_c) = P_v(T) \times F(P_c, T) \times F(w) \quad (2.1.20)$$

$$P_v(T) = 136075 \exp\left(\frac{5239.7}{273+T}\right) \quad (2.1.21)$$

$$F(P_c, T) = \exp\left(\frac{P_c M_w}{R(273+T)\rho_l}\right) \quad (2.1.22)$$

where P_c is the capillary pressure, M_w (0.018 kg/mol) is the molar mass of water, T is the absolute temperature, and R is the gas constant (8.31 J/mol/K).

Mechanical Dispersion

The mechanical dispersion is governed by Fick's law, given by

$$\mathbf{i}_\alpha^i = -(\rho_\alpha \mathbf{D}_\alpha^i \mathbf{I}) \nabla \omega_\alpha^i \quad (2.1.23)$$

where \mathbf{i}_α^i is the non-advective mass flux, with superindex i refers to species and the subindex α is refers to phase, ρ_α is the density of the phase α , \mathbf{D}_α^i is the mechanical dispersion (which is described as a function of dispersivities) tensor, and ω_α^i is the mass fraction.

2.1.4. Thermal constitutive law.

The conductive heat flux vector \mathbf{j}_c follows the Fourier's law

$$\mathbf{i}_c = -\lambda \nabla T \quad (2.1.24)$$

with



$$\lambda = \lambda_{sat} \sqrt{S_l} + \lambda_{dry} (1 - \sqrt{S_l}) \quad (2.1.25)$$

or

$$\lambda = \lambda_{sat}^{S_l} \lambda_{dry}^{(1-S_l)} \quad (2.1.26)$$

where \mathbf{i}_c is the conductive flux of heat, T is the temperature, λ is the thermal conductivity, λ_{sat} is the thermal conductivity of the water saturated porous medium, λ_{dry} is the thermal conductivity of the dry porous medium, and S_l is the degree of saturation.

Heat is also transported by liquid or gas flow and by vapour diffusion. The thermal conductivity is modified by the heat conductivities of liquid and gas, and the degree of the liquid saturation S_l as shown in equation (2.1.25) and (2.1.26). The thermal conductivity changes with porosity that affects the saturation degree S_l as well.

The thermal expansion is expressed as :

$$\Delta \varepsilon_v = 3b_s \Delta T \quad (2.1.27)$$

where ε_v is the volumetric strain, and b_s is the linear thermal expansion coefficient for the medium.

2.1.5. Geochemical formulation

In the proposed geochemical formulation, several dissolved chemical species are transported in the liquid phase through the porous medium and, simultaneously, they react among themselves (homogeneous reactions) and, also, with species present in the solid phase (heterogeneous reactions).

Chemical reactions considered in the formulation include:

- homogeneous reactions: aqueous complex formation, acid/base and oxidation/reduction,
- heterogeneous reactions: dissolution/precipitation of minerals and cation exchange.

Local equilibrium is assumed for all the chemical reactions except for dissolution/precipitation of minerals where kinetics can also be assumed. The use of one or the other of those two hypothesis must be based on the comparison between rates (or characteristic times) of concentration changes due to reactions and due to transport. Local equilibrium is the limiting case for kinetics when transport characteristic times are much higher than those of the chemical reactions.



The development of the reactive transport equations starts from the mass balance equation of each one of the species present in the medium, the final independent transport equations are obtained using the restrictions arising from the various reversible chemical reactions (local equilibrium assumption).

Let us consider the reactive transport of N chemical species in a deformable unsaturated porous medium. The transport of every one of those species can be expressed as:

$$\frac{\partial}{\partial t}(\phi S_l \rho_l c_i) + \nabla \cdot \mathbf{j}_i = R_i \quad (i = 1, \dots, N) \quad (2.1.28)$$

where c_i is the concentration of species i in mols/Kg of solution and R_i is the total production rate of species i due to chemical reactions, in mols/m³/s. \mathbf{j}_i is the total flux of species i expresses mols/m²/s. This flux is considered as the sum of advective and non-advective fluxes. Advective flux is, in turn, the sum of the movement of the liquid phase with respect to the solid phase (governed by generalized Darcy's law) and of the solid phase with respect to the reference configuration. The non-advective flux is the consequence of molecular diffusion and mechanical dispersion. For simplicity, it is assumed that the mechanical dispersion tensor is the same for all solutes. This has the advantageous consequence that electrical charge is conserved in the reactive transport equations when chemical reactions are charge balanced.

In order to make (2.1.28) valid for all species, including those in the solid phase, it is convenient to express the total flux \mathbf{j}_i as:

$$\mathbf{j}_i = \lambda_i \mathbf{j}'_i + \phi S_l \rho_l c_i \mathbf{u} \quad (2.1.29)$$

where λ_i is the mobility of species i . λ_i is 1 if the species is in the liquid phase and 0 if it is in the solid phase. \mathbf{u} is the solid phase velocity and \mathbf{j}'_i is the flux of species i with respect to the solid phase. \mathbf{j}'_i is given by:

$$\mathbf{j}'_i = \rho_l c_i \mathbf{q}_l - \mathbf{D}_l \nabla c_i \quad (2.1.30)$$

where \mathbf{q}_l is the Darcy's flux and \mathbf{D}_l the hydrodynamic dispersion tensor.

It is now necessary to introduce the reactions in local equilibrium to obtain the set of independent concentrations in the system. If N_x is the number of reversible independent reactions in a system containing N species, the number of independent chemical components is $N_c = N - N_x$. It is now possible to classify the system in N_c primary species and N_x secondary species. Reversible reactions between the two types of species are expressed as:

$$A_i = \sum_{j=1}^{N_c} \nu_{ij} A_j \quad (i = 1, \dots, N_x) \quad (2.1.31)$$



where A_j and A_i are the chemical formulas of the primary and secondary species respectively and v_{ij} the number of mols of the primary species j in a mol of the secondary species i . It should be noted that the classification of the species into primary and secondary ones is not unique.

Using the properties of the reversible reactions (2.1.31), it is possible to derive the basic transport equation (2.1.32):

$$\frac{\partial}{\partial t}(\phi S_l \rho_l U_j) + \nabla \cdot \begin{pmatrix} \rho_l U a_j \mathbf{q}_l - \mathbf{D}_l \nabla U a_j \\ + \phi S_l \rho_l U_j \dot{\mathbf{u}} \end{pmatrix} + \sum_{m=1}^{N_m} v_{jm} r_m = 0 \quad (j = 1, \dots, N_c) \quad (2.1.32)$$

$$U_j = C_j + \sum_{i=1}^{N_x} v_{ij} X_i \quad (i = 1, \dots, N_c) \quad (2.1.33)$$

$$U a_j = \lambda_j C_j + \sum_{i=1}^{N_x} v_{ij} \lambda_i X_i \quad (i = 1, \dots, N_c) \quad (2.1.34)$$

where U_j is the total analytical concentration and $U a_j$ is the total aqueous concentration of the primary species j . C_j and X_i are the concentrations of the primary and secondary species respectively. λ_j and λ_i are the mobilities of the primary and secondary species. r_m is the rate of precipitation or dissolution of mineral m under kinetics conditions and N_m is the number of minerals in kinetics conditions. v_{jm} is the number of moles of primary species j in a mol of mineral m .

A possible way to solve equation (2.1.32) is taking the concentrations of primary and secondary species C_j and X_i as unknowns. The additional N_x required equations are supplied by the geochemical model (e. g. mass action law). In the present formulation, the total analytical concentrations U_j are the unknowns of the transport equations (2.1.32), and $U a_j$ and r_m are considered non-linear functions of U_j . The link between the unknowns U_j and the dependent variables $U a_j$ and r_m is the chemical equilibrium model. This type of unknown exhibits the interesting property of being independent of chemical equilibrium. Total analytical concentration changes in time are exclusively due to transport and kinetics reactions.

2.2. Posiva/Marintel (FreeFEM++)

FreeFEM++ is a finite element code developed by Marintel. It is applied to THMC processes in 2D problems.

2.2.1. Mathematical formulation

- Momentum balance of the medium:

$$\nabla \cdot \boldsymbol{\sigma} = \mathbf{0}$$



(2.2.1)

Body force neglected

- Mass balance of water:

$$\frac{dm^w}{dt} + \text{div} \mathbf{w}^w = 0 \quad (2.2.2)$$

where: m^w is the mass of water and \mathbf{w}^w is the mass flux vector of water.

- Thermal equation:

$$\text{div} \mathbf{q} = 0 \quad (2.2.3)$$

where \mathbf{q} is heat flux vector.

2.2.2. Mechanical constitutive law.

The equation of state for the stress \mathbf{s} and Gibb's potential g^w can be written in the form:

$$d\sigma = \left(K - \frac{2}{3} G \right) d\varepsilon \mathbf{I} + 2G \mathbf{e} - (Mb)^w \frac{dm^w}{\rho^w} \mathbf{1} \quad (2.2.4)$$

$$dg^w = -\frac{1}{\rho^w} (Mb)^w d\varepsilon + \frac{1}{\rho^w} M^w \frac{dm^w}{\rho^w}, k \in S \quad (2.2.5)$$

These are the undrained equations, because K is the bulk modulus in evolution with constant moisture content. G is the shear modulus, M^w is the Biot modulus and b^w is the Biot coefficient and ρ^w is the density of liquid water. The thermal expansion term is neglected, because the hydration swelling is stronger than thermal swelling.

Re-writing the above equations:

$$d\sigma + \rho^w b^w dg^w \mathbf{I} = \left(K^0 - \frac{2}{3} G \right) d\varepsilon \mathbf{I} + 2G \mathbf{e} - A^0 \mathbf{I} dT \quad (2.2.6)$$

$$M^w \frac{dm^w}{\rho^w} = - (Mb)^w + \rho^w dq^w - 3(\alpha M)^w dT, k \in S \quad (2.2.7)$$

where $K^0 = K - \sum_{k \in S} b^k (Mb)^k$

Equations (2.2.6) and (2.2.7) are called drained equations, because K^0 is the bulk modulus when the Gibb's function is held constant but mass contents can change.



According to observation (Börgesson et al. 1995) the classical effective pressure

$$p_c^* = -\frac{1}{3} \text{trace} \boldsymbol{\sigma} - p^w \quad (2.2.8)$$

Behaves according:

$$\frac{p_c^*}{p_{ref}^*} = \left(\frac{e}{e_{ref}} \right)^{-1/\beta} \quad (2.2.9)$$

where b , p_{ref}^* and e_{ref} are materials constant. Since in linear approximation the void ratio is related to dilation by: $e = (1 + \varepsilon) \exp(\varepsilon) - 1$

The classical undrained bulk modulus is determined by:

$$K_c^0 = \frac{p^* (1 + e_0) \exp(\varepsilon)}{\beta e_0} \left(\frac{(1 + e_0) \exp(\varepsilon) + 1}{e_0} \right)^{-(1+\beta)/\beta} \quad (2.2.10)$$

2.2.3. Moisture conduction.

$$w^m = D\varepsilon \nabla \varepsilon - D_m \nabla m^w - D_T \nabla T \quad (2.2.11)$$

where D_e , D_m , D_T are the moisture diffusion.

The hydraulic conductivity k_{sat}^* of a saturated media is defined as:

$$\frac{w^w}{\rho_w} = -k_{sat}^* \frac{\nabla p_L^w}{\rho^w g} \quad (2.2.12)$$

where p_L^w is the pore water pressure of the fluid phase

The unsaturated hydraulic conductivity is:

$$k^* = (S_r)^\delta k_{sat}^* \quad (2.2.13)$$

The relation between hydraulic conductivity and moisture diffusion coefficient D_m can be directly calculated from:

$$D_m = \frac{k_{sat}^*}{\rho^w g} (S_r)^\delta M^w \quad (2.2.14)$$

The coefficients D_m and $D_{e\varepsilon}$ are simply related by Biot coefficient,

$$D_{\varepsilon} = b^w D_m \quad (2.2.15)$$

Considering the following equation of suction, then D_m is calculated by equation (2.2.17):

$$s = s_0 \exp\left(-\frac{m^w}{C\rho_d}\right) \quad (2.2.16)$$

$$D_m = \frac{s_0 k_{sat}^* (S_r)^\delta}{g C \rho_d} \exp\left(-\frac{m^w}{C\rho_d}\right) \quad (2.2.17)$$

The thermal moisture conduction parameter D_T can be derived from data for water vapour transport given in (Börgesson et al, 1995)

$$D_T^w = 0, \text{ for } S_r \leq 0.15 \text{ or } S_r \geq 0.95 \quad (2.2.18)$$

$$D_T^w = D_{Tr} D_m^w, \text{ for } 0.6 \leq S_r \leq 0.8 \quad (2.2.19)$$

$$D_T^w = D_{Tr} \frac{S_r - 0.2}{0.4} D_m^w, \text{ for } 0.2 \leq S_r \leq 0.6 \quad (2.2.20)$$

$$D_T^w = D_{Tr} \frac{0.95 - S_r}{0.15} D_m^w, \text{ for } 0.8 \leq S_r \leq 0.95 \quad (2.2.21)$$

where D_{TR} is a material parameter.

2.2.4. Thermal behaviour.

The heat flow process is viewed as a heat conduction process governed by

$$C_v \frac{dT}{dt} - \frac{\partial}{\partial x_i} \left(\lambda \frac{\partial T}{\partial x_i} \right) = Q \quad (2.2.22)$$

$$\lambda = \lambda_1 + \frac{\lambda_0 - \lambda_1}{1 + \exp[(S_r - x_0)/d_x]} \quad (2.2.23)$$

where C_v is the volumetric heat capacity, λ is the heat conduction coefficient, Q is the local heat production (caused by chemical reactions, not yet implemented and probably

not important), λ_0 is the heat conduction coefficient at $S_r = x_0$, λ_1 is the heat conduction coefficient at $S_r = 1$, and d_x is the shape parameter.

Heat convection is neglected. In most applications the heat storage term $C_v dT/dt$ can also be neglected.

2.3. KTH (ROLG)

ROLG is a finite element program formulated in 3D. The objective of this code is the simulation of coupled thermo-hydro-mechanical processes for geological media. Its formulation is based on Biot's poroelasticity theory, where the pore pressure, displacements and temperature are unknowns. The formulation also considers the water flow due to thermal phenomena and the swelling of the bentonite due to water content changes.

2.3.1. Mechanical behaviour.

The equation of motion of the bentonite includes the effects of heat and fluid pressure on the deformation process, governed by

$$\nabla \cdot \left(\mathbf{D} : \frac{\partial \boldsymbol{\varepsilon}}{\partial t} \right) + \nabla \cdot \left(-\mathbf{I} \alpha \frac{\partial P}{\partial t} \right) + \nabla \cdot \left(-\mathbf{D} : \mathbf{I} \beta \frac{\partial T}{\partial t} \right) + \nabla \cdot \left(-\mathbf{I} \frac{\partial \sigma_{sw}}{\partial t} \right) + \frac{\partial \mathbf{F}}{\partial t} = 0 \quad (2.3.1)$$

where \mathbf{D} is the tensor of elasticity as a function of the Young's modulus E and Poisson's ratio ν in the theory of elasticity, $\boldsymbol{\varepsilon}$ is the total strain tensor, \mathbf{I} is the identity tensor, α the Biot coefficient ($\alpha = 0$ for unsaturated media and $\alpha = 1 - K_d/K_g$ for saturated media where K_g is the bulk modulus of solid grain, K_d the drained bulk modulus of material), P the pore pressure, β the thermal expansion coefficient, \mathbf{F} the body force vector, and σ_{sw} is the swelling pressure which is calculated as a function of volumetric water content:

$$\sigma_{sw} = \sigma_{sw \max} \sqrt{S_r} \quad (2.3.2)$$

The linear and isotropic elasticity is used as constitutive for the bentonite.

2.3.2. Hydraulic behaviour.

Two different equations for fluid flow are considered depending on zones that are saturated or unsaturated. The effect of the mechanical coupling is considered by the volumetric strain. For saturated zones, the moisture diffusion is governed by the Darcy's law:

$$\frac{\partial P}{\partial t} = \frac{BK}{\alpha(1-\alpha B)} \nabla \cdot \left(\frac{\mathbf{k}}{\mu} (\nabla P - \rho_w \mathbf{g}) \right) - \frac{BK}{1-\alpha B} \frac{\partial \varepsilon_b}{\partial t} \quad (2.3.3)$$



And for unsaturated zones a vapour diffusion term driven by thermal gradient is added:

$$C \frac{\partial P'}{\partial t} = \nabla \cdot \left(\frac{k_r \mathbf{k}}{\mu} (\nabla P' - \rho_w \mathbf{g}) \right) - S_r \alpha \frac{\partial \varepsilon_b}{\partial t} + \nabla \cdot (D_{TV} (\nabla T)) \quad (2.3.4)$$

where P is the water pressure in saturated zone, B is the Skempton coefficient, K is the macroscopic bulk modulus, \mathbf{k} is the permeability tensor in saturated state, μ is the fluid viscosity, which is the function of temperature and can be expressed as:

$$\mu = (0.0001T^4 - 0.0047 T^3 + 0.0802 T^2 - 0.6313 T + 2.3181) \times 10^{-6}$$

ε_b the volumetric strain, ρ_w the fluid density, \mathbf{g} the gravitational acceleration vector, S_r the saturated degree, k_r the relative permeability, which is function of the saturated degree and can be expressed as $k_r = S_r^3$, D_{TV} the thermal water diffusivity, which can be obtained from following formula:

$$D_{TV} = 7.0 \times 10^{-12} \sin^6 \left(\frac{S_r \pi}{0.5} \right)$$

P' is the suction in unsaturated zone, respectively, the relation between suction and degree of saturation can be defined as water retention curve, and can be written as:

$$S_r = \left[1 + (5.2 \times 10^{-5} P')^{1.7} \right]^{-0.41176}$$

C is obtained from water retention curve as: $C = -\frac{\partial S_r}{\partial P'}$

2.3.3. Thermal behaviour.

The heat conduction and convection are considered. The effect of the mechanical deformation is also included. The governing equation is:

$$\rho c \frac{\partial T}{\partial t} + \nabla \cdot (-k_r \mathbf{k}_T \nabla T) + \nabla \cdot \left(\rho_w c_w T \left(-k_r \frac{\mathbf{k}}{\mu} (\nabla P' - \rho_w \mathbf{g}) \right) \right) - Q + 3K\beta(T - T_a) \frac{\partial \varepsilon_b}{\partial t} = 0 \quad (2.3.5)$$

where $\rho = \rho_d + (\rho_{sa} - \rho_d) S_r$; ρ_d and ρ_{sa} are density of poroelastic in dry and saturated state respectively, c is the specific heat capacity of the poroelastic media, which is a function of the density of water and water content given as $c = \rho_w \frac{80.0 + 4.2w}{100 + w}$

c_w is the specific heat capacity of the fluid (water), \mathbf{K}_T is the thermal conductivity tensor at saturated state, k_{rt} is the relatively thermal conductivity coefficient, which is a

function of degree of saturated given as $k_{rt} = A \left(\frac{A_1 - A_2}{1 + e^{(S_r - x_0)/dx}} + A_2 \right)$

with $A = 0.7943$ $A_1 = 0.57$ $A_2 = 1.28$ $x_0 = 0.65$ $dx = 0.1$

P the water pressure in saturated zone or suction in unsaturated zone (P') and Q is the heat resource.



2.4. Quintessa (QPAC-EBS)

QPAC-EBS is a modular multi-physics code developed by Quintessa. It uses compartments to discretize the system and can represent coupled non-linear processes. Partial differential equations (PDEs) are discretized onto those compartments, and the finite volume method is generally employed. A general-purpose solver is used for the solution of systems of ordinary differential equations with associated algebraic constraints. Any problem dimension can be considered, including 3D.

2.4.1. Mechanical behaviour.

The effective stress σ_{en} (Pa) in the solid in a given direction n is taken to be the stress less the pressure in the pores and an allowance for vertical stresses due to gravitation:

$$\sigma_{en} = \sigma_n - P \quad (2.4.1)$$

where: σ_{en} is the effective stress (Pa), σ_n is the stress (Pa), P is the pressure in the pores (Pa)

For viscoelasticity, the constitutive relations are given by Maxwell model:

$$\frac{d\varepsilon_n}{dt} = \frac{\sigma_{\Sigma n}}{\mu} + \frac{1}{E} \frac{d\sigma_{en}}{dt} \quad (2.4.2)$$

$$\sigma_{\Sigma x} = \sigma_{ex} - \nu(\sigma_{ey} + \sigma_{ez}) \quad (2.4.3)$$

$$\sigma_{\Sigma y} = \sigma_{ey} - \nu(\sigma_{ez} + \sigma_{ex})$$

$$\sigma_{\Sigma z} = \sigma_{ez} - \nu(\sigma_{ey} + \sigma_{ex})$$

where ε_n is the strain (-), $\sigma_{\Sigma n}$: is the net effective stress in direction n , E is Young's Modulus (Pa), μ is the viscosity of the material (Pa s), and ν is Poisson's ratio (-).

Displacements of compartments and their associated interfaces are represented through a kinetic description of compartment deformation that reflects the calculated compartmental deformations. In this approach fluxes of displacement are moved through the model such that internal interfaces lie on the boundaries of compartments and respectively prescribed boundaries. The displacements are accumulated in each compartment along each principal axes:

$$q_{d,n} = \frac{\left((l_{n,i} - l_{n,c}) - l_{n,h} (1 - \varepsilon_n) \right) \xi}{\tau} \quad (2.4.4)$$

where $q_{d,n}$ is the displacement flux (m s^{-1}), $l_{n,i}$ is the location of the interface along principal axis n , $l_{n,c}$ is the half length of the compartment along principal axis n , ξ is a correction parameter taking the value 1 to -1 to take into account the orientation of the interface relative to the principal axis. The characteristic timescale for all such kinetic balancing is set through the parameter τ .

The interfaces are constrained always to lie on one of the compartment boundaries hence the above 'flux' will tend to zero as the displacements reflect the stress-strain relations in the model. This ensures that the displacements of interfaces are always consistent with the calculated strains and the bulk discontinuous displacements of compartments. The displacement 'model' is coupled back to the deformation model such that prescribed displacements on interfaces can be defined along boundaries.

2.4.2. Hydraulic behaviour.

The mass balance of the fluid equation is:

$$\frac{\partial}{\partial t} (\theta \rho_i S_i) = -\nabla \cdot (\rho_i \mathbf{u}_i) + q_i \quad (2.4.5)$$

where θ is the porosity of the porous medium (-), ρ_i is the density of fluid i (kg m^{-3}), S_i is the saturation of the fluid i (where the total over all fluids is unity), p_i is the pressure for fluid i (Pa) (-), q_i is the source or sink amount of fluid i ($\text{kg m}^{-3} \text{s}^{-1}$), \mathbf{u}_i is the Darcy velocity vector of fluid i (m s^{-1}),

$$\mathbf{u}_i = -\frac{k_i}{\mu_i} \nabla (p_i + \rho_i g z)$$

where g is the acceleration due to gravity (ms^{-2}), k_i the effective permeability for fluid i (m^2), μ_i is the viscosity of fluid i (Pa s), and z is the vertical coordinate (measured positive upwards) (m).

The effective permeability tensor of the porous media for fluid i is expressed as a scaling of the intrinsic permeability of the medium by a relative permeability function.

$$k_i = k_{r,i}(S_i) k(\theta) \quad (2.4.6)$$

where k is the intrinsic permeability of the medium (m^2), $k_{r,i}$ is the relative permeability function (-).

At the contact interface between two fluids there is a balance between the forces that act on the molecules within each fluid. The contact pressure is referred to as the capillary pressure:

$$p_{c_j} = p_{g_j} - p_w$$

where p_{c_j} is the capillary pressure for non-wetting phase j (Pa), p_{g_j} is the pressure in non-wetting phase j (Pa), p_w is the pressure in the wetting phase (Pa).

Vapour transport

The representation of this process is closely to the thermal evolution of the system. Following the approach of Claesson and Sällfors (2005) the water vapour flux is given by:

$$g_{vap} = -AD_s(S) \frac{\partial \rho_v}{\partial r} \quad (2.4.7)$$

where g_{vap} is the vapour mass flux (kg s^{-1}), A is the interface area (m^2), $D_v(S)$ is a diffusion coefficient ($\text{m}^2 \text{s}^{-1}$), ρ_v is the vapour density (kg m^{-3}). The diffusion coefficient $D_s(S)$ is related to its unsaturated value, $D_v(0)$, by a scaling based on the water saturation, S_w :

$$D_s(S) = D_v(0)(1 - S_w) \quad (2.4.8)$$

The water vapour density is given by:

$$\rho_v = h \rho_{vs} \quad (2.4.9)$$

The saturated water vapour density, ρ_{vs} , is given by an empirical formula (Rutqvist et al., 2003)

$$\rho_{vs} = 10^{-3} \exp\left(19.891 - \frac{4975.9}{T}\right) \quad (2.4.10)$$

The relative humidity h was defined using the following relationship (Engel et al., 2003)

$$h = \exp\left(\frac{-\Psi M_{vapour}}{\rho_w RT}\right) \quad (2.4.11)$$

where Ψ is the suction pressure (Pa), M_{vapour} is the molar mass of vapour (kg mol^{-1}), R is the gas constant, and T is the water temperature (K).

A default relationship for suction pressure and fraction of water as vapour in betonite is also provided (Rutqvist, et al. 1999):

$$S_w(1 - S_v) - [1 - (\Psi/\Psi_d)]^{l_d} \left[1 + (\Psi/P_0)^{1/(1-l_0)} \right]^{-l_0} = 0 \quad (2.4.12)$$

where S_v is the fraction of water as vapour, Ψ_d is the suction pressure at zero saturation (Pa), P_0 is the air entry pressure (Pa), and l_d and l_0 are fitting parameters (-).

2.4.3. Thermal behaviour

The governing equations for thermal conduction are written in the following form:

$$\frac{\partial Q_H}{\partial t} = F_{HC} + P \quad (2.4.13)$$

$$Q_H = V\rho cT \quad (2.4.14)$$

$$F_{HC} = A\nabla \cdot (\Gamma\nabla T) \quad (2.4.15)$$

where T is the temperature (K), ρ is the density of the medium (kg m^{-3}), c is the specific heat capacity ($\text{J kg}^{-1} \text{K}^{-1}$), Γ is the thermal conductivity ($\text{W m}^{-1} \text{K}^{-1}$), V is the compartment volume (m^3), F_{HC} is the conductive heat flux (J s^{-1}), and A is the interface area between the compartments (m^2).

Convection of heat via the movement of fluid in the porous medium adds a contribution of the heat flux on an interface.

$$F_{HF} = Aq_F\rho_F c_F T \quad (2.4.16)$$

where F_{HF} is a transfer of heat flux (J s^{-1}), q_F is the Darcy velocity across the interface (m s^{-1}), ρ_F is the fluid density (kg m^{-3}), c_F is the specific heat capacity of the fluid ($\text{J kg}^{-1} \text{K}^{-1}$).

2.4.4. Other phenomena considered

Kinetic dissolution:

To model kinetic dissolution, the dissolved phases must be treated as evolving variables and the dissolution rate is represented as a source/sink term between free and dissolved phases. Dissolved fluid is transported by the solvent, so the evolution equation for dissolved phase is:

$$\frac{\partial}{\partial t} (c_{g,j}^{diss} \theta \rho_w S_w) = -\nabla \cdot (c_{g,j}^{diss} \rho_w \mathbf{u}_w) + q_{gj} \quad (2.4.17)$$

$$q_{gj} = R_{diss,j} + \hat{q}_{gj} \quad (2.4.18)$$

$$R_{diss,j} = \lambda \theta \rho_w S_w (c_{g,j}^{Henry} - c_{g,j}^{diss}) \quad (2.4.19)$$

where λ is the dissolution rate constant (y^{-1}), $c_{g,j}^{Henry}$ the concentration determined using Henry's law ($\text{mol} \cdot \text{m}^{-3}$), $c_{g,j}^{diss}$ the instantaneous concentration calculated in the model ($\text{mol} \cdot \text{m}^{-3}$), S_w is the water saturation (-), and ρ_w is the water density ($\text{kg} \cdot \text{m}^{-3}$).

2.5. CU (COMPASS)

COMPASS is a computational code developed by Cardiff University, UK. The finite element method is used for the spatial discretization and finite difference method is used to solve the temporal discretization. This code is able to simulate thermo-hydro-mechanical and chemical problems in 1D, 2D and 3D. It also includes a multi-component geochemistry formulation.

2.5.1. Mechanical behaviour.

The formulation is presented for the more general case of unsaturated soil. Under saturated conditions the net mean stress becomes effective stress in this code. Thermal stresses are implicitly addressed in the stress-strain equations. The equation of motion of the bentonite considered is written as:

$$\mathbf{P} d\sigma_i'' + m_i \mathbf{P} du_a + db_i = 0 \quad (2.5.1)$$

where σ_i'' : the net stress $d\sigma_i'' = d(\sigma - m_i u_i)$, u_a : pore air pressure, b_i : body force, \mathbf{P} : strain matrix, m_i : unit vector as defined below.

2.5.2. Mechanical constitutive law.

Non-linear Elastic State model

The total elastic strain (in incremental form) is defined as the sum

$$d\varepsilon^e = d\varepsilon_p^e + d\varepsilon_s^e + d\varepsilon_T^e \quad (2.5.2)$$

where ε^e is the total elastic strain, ε_p^e is the elastic strain due to net mean stress (over air pressure), ε_s^e is the elastic strain due to suction, ε_T^e is the elastic strain due to temperature.

The elastic strain due to mean stress is defined as:

$$d\varepsilon_p^e = \frac{m_i}{\eta} \frac{1}{\nu_0} \frac{\partial e}{\partial p} dp \quad (2.5.3)$$

where $\eta = 2$ for 2D problems and 3 for 3D problems, e the void ratio, ν_0 the initial specific volume of the bentonite, respectively.

The elastic strain due to suction is defined as

$$d\varepsilon_s^e = \frac{m_i}{\eta} \frac{1}{\nu_0} \frac{\partial e}{\partial s} ds \quad (2.5.4)$$

where s is the suction at temperature T .

The elastic strain due to temperature is defined as

$$d\varepsilon_T^e = \left[\alpha_T + \frac{1}{\nu_0} \frac{\partial e}{\partial s_r} \frac{\partial s_r}{\partial T} \right] \frac{m_i}{\eta} dT \quad (2.5.5)$$

where α_T is the coefficient of thermal expansion of the bentonite, and s_r is the suction at reference temperature respectively.

$$s_r = \frac{\xi_r}{\xi} s \quad (2.5.6)$$

$$\xi = 0.1171 - 0.0001516T \quad (2.5.7)$$

where ξ and ξ_r are the surface energy at the actual temperature T and reference temperature T_r , respectively.

The deviatoric strain is defined as:

$$d\varepsilon_q^e = \frac{dq}{3G} \quad (2.5.8)$$

where q is the deviatoric stress and G is the shear modulus.

A linear stress-strain relation is then defined as:

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$$d\sigma_i^n = \mathbf{D} \left[d\varepsilon^e - d\varepsilon_s^e - d\varepsilon_T^e \right] \quad (2.5.9)$$

where σ_i^n is the net mean stress as defined before and \mathbf{D} is the standard elasticity matrix. Equation (2.5.9) can be explicitly expressed as:

$$d\sigma_i^n = \mathbf{D} \left[d\varepsilon^e - A_s \frac{\partial s_r}{\partial s} ds - \left(A_T + A_s \frac{\partial s_r}{\partial T} \right) dT \right] \quad (2.5.10)$$

with the suction vector defined as

$$A_s = \frac{m_i}{\eta} \frac{1}{v_0} \frac{\partial e}{\partial s_r} \quad (2.5.11)$$

and the thermal vector given by

$$A_T = \frac{m_i}{\eta} \alpha_T \quad (2.5.12)$$

The parameter e used in equations (2.5.3, 2.5.4 and 2.5.5) are defined by a state surface relation given by

$$e = e_o + a \ln p + b \ln s + c \ln p \ln s + \alpha_T \Delta T \quad (2.5.13)$$

where p is the net mean stress and a , b and c are the state surface coefficients, respectively.

The governing differential equation (equations of motion) with the above non-linear elastic model can then be written as:

$$C_{ul} du_l + C_{uT} dT + C_{ua} du_a + C_{uu} d\mathbf{u} + db_i = 0 \quad (2.5.14)$$

with

$$C_{ul} = \mathbf{P} \mathbf{D} A_s \frac{\partial s_r}{\partial s}$$

$$C_{uT} = \mathbf{P} \mathbf{D} \left(-A_T - A_s \frac{\partial s_r}{\partial T} \right)$$

$$C_{ua} = -\mathbf{P} \mathbf{D} A_s \frac{\partial s_r}{\partial s} - m_i \mathbf{P}$$

$$C_{uu} = \mathbf{P} \mathbf{D} \mathbf{P}^T$$

Elasto-plastic model

An elasto-plastic model based on critical state concept and the Barcelona Basic Model is used for the bentonite behaviour for WP4. The total strain, ε , (in incremental form) is defined as the sum

$$d\varepsilon = d\varepsilon_p^e + d\varepsilon_s^e + d\varepsilon_T^e + d\varepsilon^p \quad (2.5.15)$$

where ε^e is the total elastic strain, ε_p^e is the elastic strain due to net mean stress (over air pressure), ε_s^e is the elastic strain due to suction, ε_T^e is the elastic strain due to temperature, ε^p is the plastic strain = $\varepsilon_p^p + \varepsilon_s^p$, ε_p^p is the plastic strain due to net mean stress and ε_s^p is the plastic strain due to suction.

The elastic strain due to mean stress is defined as

$$d\varepsilon_p^e = -\frac{m_i \kappa}{\eta \nu_0} \frac{dp}{p} \quad (2.5.16)$$

The elastic strain due to suction is defined as

$$d\varepsilon_s^e = -\frac{m_i \kappa_s}{\eta \nu_0} \frac{ds}{(s + p_{atms})} \quad (2.5.17)$$

The elastic strain due to temperature is defined as

$$d\varepsilon_T^e = \left[\frac{\alpha_T}{\nu_0} - \frac{\kappa_s}{\nu_0} \frac{1}{(s + p_{atms})} \frac{\partial s_r}{\partial T} \right] \frac{m_i}{\eta} dT \quad (2.5.18)$$

The plastic strain due to mean stress is defined as

$$d\varepsilon_p^p = \frac{m_i}{\eta} \chi_1 \frac{dQ_1}{dp} \quad (2.5.19)$$

The plastic strain due to suction is defined as

$$d\varepsilon_s^p = \frac{m_i}{\eta} \chi_2 \frac{dQ_2}{ds} \quad (2.5.20)$$

where κ is the stiffness parameter for changes in net mean stress in the elastic region, κ_s is the stiffness parameter for changes in suction in the elastic region, p_{atms} has been added to avoid infinite values of strain as suction approaches zero, α_T is the coefficient of thermal expansion, Q_1 and Q_2 are the plastic potentials, and χ_1 and χ_2 are plastic

multipliers which are determined through plastic consistency conditions. Parameters p , v_0 , m_i , η , s , s_r and T are defined before.

The plastic potential can be written as

$$Q_1 = \alpha_q q^2 - M^2(p + p_s)(p_0 - p) \quad (2.5.21)$$

and

$$Q_2 = s - s_0 \quad (2.5.22)$$

where Q_1 corresponds to the LC flow rule, Q_2 corresponds to the SI flow rule, α_q is a constant derived from the 'at rest' stress state for which there is zero lateral deformation, M is the slope of the critical state line, p_s is the parameter controlling suction effect on cohesion, p_0 is the pre-consolidation stress at a suction s and s_0 is the critical value of suction (suction hardening parameter), respectively.

The pre-consolidation stress varies with suction, determining the collapse behaviour of the soil during wetting, according to the following relation

$$\left(\frac{p_0}{p_c} \right) = \left(\frac{p_0^*}{p_c} \right)^{\left(\frac{\lambda(0) - \kappa}{\lambda(s) - \kappa} \right)} \quad (2.5.23)$$

where p_0^* is the preconsolidation stress of saturated soil, p_c is the reference stress, $\lambda(s)$ is the stiffness parameter for changes in net mean stress for virgin states of the soil and $\lambda(0)$ is the stiffness parameter for changes in net mean stress for virgin states of saturated soil.

Assuming that the elastic strain increment is equal to zero, the resulting expression for α_q in equation (5.20) is given as follows:

$$\alpha_q = \frac{M(M-9)(M-3)}{6(6-M)} \left\{ \frac{1}{1 - [\kappa/\lambda(0)]} \right\} \quad (2.5.24)$$

The elastic strain due to deviatoric stress is defined as

$$d\varepsilon_q^e = \frac{dq}{3G} \quad (2.5.25)$$

The plastic strain due to deviatoric stress is defined as

$$d\varepsilon_q^p = \chi_1 \frac{dQ_1}{dq} \quad (2.5.26)$$

where q is the deviatoric stress and G is the shear modulus.

The resultant stress-strain relation is then

$$d\sigma'' = \mathbf{D}_{ep} \left[d\varepsilon - d\varepsilon_s^e - d\varepsilon_T^e - d\varepsilon^p \right] \quad (2.5.27)$$

where \mathbf{D}_{ep} is an elasto-plastic matrix that is defined as

$$\mathbf{D}_{ep} = \mathbf{D} - \frac{\mathbf{D} \frac{\partial Q_1}{\partial \sigma} \frac{\partial F_1}{\partial \sigma} \mathbf{D}}{\mathbf{A} + \left(\frac{\partial Q_1}{\partial \sigma} \right)^T \mathbf{D} \frac{\partial F_1}{\partial \sigma}} \quad (2.5.28)$$

where \mathbf{D} is the elastic matrix, Q_1 the plastic potential, F_1 the yield function, σ the total stress and \mathbf{A} is the plastic modulus, respectively. F_1 is defined as:

$$F_1(p, q, s, p_0^*) = q^2 - M^2(p + p_s)(p_0 - p) = 0 \quad (2.5.29)$$

where M is the slope of the critical state line, p_s is the parameter controlling suction effect on cohesion, p_0 is the pre-consolidation stress at a suction s , p_0^* is the saturated pre-consolidation stress, and q is the deviatoric stress.

The governing equations of motion with the elasto-plastic model can then be written as

$$C_{ul} du_l + C_{uT} dT + C_{ua} du_a + C_{uu} d\mathbf{u} - \mathbf{PD}_{ep} \varepsilon_s^p + db_i = 0 \quad (2.5.30)$$

with

$$C_{ul} = \mathbf{PD}_{ep} A_s$$

$$C_{uT} = \mathbf{PD}_{ep} \left(-A_T - A_s \frac{\partial s_r}{\partial T} \right)$$

$$C_{ua} = -\mathbf{PD}_{ep} A_s - m_i \mathbf{P}$$

$$C_{uu} = \mathbf{PD}_{ep} \mathbf{P}^T$$

Also included in the COMPASS code is a linear elastic model that requires only the Young's modulus E , shear modulus G and/or Poisson's ratio ν as constants.

2.5.3. Hydraulic behaviour.

The theoretical formulation is the Darcy's law for liquid flow, osmotic flow and vapour flow is based on Philip and de Vries (1957) and Ewen and Thomas (1989).

Mass balance equation of water:

$$C_{ll} \frac{\partial u_l}{\partial t} + C_{lr} \frac{\partial T}{\partial t} + C_{la} \frac{\partial u_a}{\partial t} + C_{lu} \cdot \frac{\partial \mathbf{u}}{\partial t} = \nabla \cdot [K_{ll} \nabla u_l] + \nabla \cdot [K_{lr} \nabla T] \quad (2.5.31)$$

$$+ \nabla \cdot [K_{la} \nabla u_a] + \nabla \cdot \sum_{j=1}^{nc} \rho_l K_{l_{cd}}^j \nabla c_d^j + J_l$$

with

$$C_{ll} = -n(\rho_l - \rho_v) \frac{\partial S_l}{\partial s} - n(1 - S_l) \rho_0 \frac{\partial h}{\partial s}$$

$$C_{lr} = n(\rho_l - \rho_v) \frac{\partial S_l}{\partial T} + n(1 - S_l) \left(h \frac{\partial \rho_0}{\partial T} + \rho_0 \frac{\partial h}{\partial T} \right)$$

$$C_{la} = n(\rho_l - \rho_v) \frac{\partial S_l}{\partial s} + n(1 - S_l) \rho_0 \frac{\partial h}{\partial s}$$

$$C_{lu} = (S_l \rho_l + (1 - S_l) \rho_v) \mathbf{m}_l^T \mathbf{P}$$

$$K_{ll} = \rho_l \left[\frac{k_l}{\gamma_l} - \frac{D_{atms} v_v n}{\rho_l} \left(\rho_0 \frac{\partial h}{\partial s} \right) \right]$$

$$K_{lr} = \rho_l \frac{D_{atms} v_v n (\nabla T)_a}{\rho_l \nabla T} \left(h \frac{\partial \rho_0}{\partial T} + \rho_0 \frac{\partial h}{\partial T} \right)$$

$$K_{la} = \rho_v k_a + \rho_l \left[\frac{D_{atms} v_v n}{\rho_l} \left(\rho_0 \frac{\partial h}{\partial s} \right) \right]$$

$$J_l = \rho_l \nabla \cdot (K_l \nabla z)$$

where u_l is the pore water pressure, u_a is the pore air pressure, \mathbf{u} is the displacement vector, T is the temperature, nc is the number of chemical species, $K_{l_{cd}}^j$ is the permeability with respect to chemical solute gradient, c_d^i is the dissolved concentration of chemical component i , n is the porosity, ρ_l is the density of pore liquid moisture, ρ_v is the density of water vapour, ρ_0 is the saturated soil water vapour density, S_l is the degree of saturation of pore liquid, s is the suction at a temperature T , h is the relative humidity, \mathbf{m} is a unit vector, \mathbf{P} is the strain-displacement matrix, k_l is the effective permeability of pore liquid, γ_l is the unit weight of liquid moisture, D_{atms} is the molecular diffusivity of vapour through air, v_v is the mass flow factor, $(\nabla T)_a / \nabla T$ is

the ratio of the microscopic temperature gradient in pore space to the macroscopic temperature gradient, k_a is the effective permeability of pore air, k_l is the unsaturated hydraulic conductivity, and z is the global vertical coordinate.

Mass balance of dry air:

$$C_{al} \frac{\partial u_l}{\partial t} + C_{aT} \frac{\partial T}{\partial t} + C_{aa} \frac{\partial u_a}{\partial t} + C_{au} \cdot \frac{\partial \mathbf{u}}{\partial t} = \quad (2.5.32)$$

$$\nabla [K_{al} \nabla u_l] + \nabla [K_{aa} \nabla u_a] + \nabla \cdot \sum_{j=1}^n K_{a_{cd}}^j \nabla c_d^j + J_a$$

with

$$C_{al} = -n\rho_{da}(H_s - 1) \frac{\partial S_l}{\partial s} + n(S_a + H_s S_l) \frac{R_v}{R_{da}} \left(\rho_0 \frac{\partial h}{\partial s} \right)$$

$$C_{aT} = n\rho_{da}(H_s - 1) \frac{\partial S_l}{\partial T} - n(S_a + H_s S_l) \left(\frac{\rho_a}{T} - \frac{R_v}{R_{da}} \left(h \frac{\partial \rho_0}{\partial T} + \rho_0 \frac{\partial h}{\partial T} \right) \right)$$

$$C_{aa} = n\rho_{da}(H_s - 1) \frac{\partial S_l}{\partial s} + n(S_a + H_s S_l) \left(\frac{1}{R_{da} T} - \frac{R_v}{R_{da}} \rho_0 \frac{\partial h}{\partial s} \right)$$

$$C_{au} = \rho_{da} (S_a + H_s S_l) \mathbf{m}_i^T \mathbf{P}$$

$$K_{al} = \frac{\rho_{da} H_s}{\gamma_l} k_l$$

$$K_{aa} = \rho_{da} k_a$$

$$K_{a_{cd}}^j = \rho_{da} H_s K_{l_{cd}}^j$$

$$J_a = \rho_{da} H_s \nabla \cdot (k_l \nabla z)$$

where ρ_{da} is the density of dry air, H_s is Henry's volumetric coefficient of solubility, S_a is the degree of saturation of pore air, R_v is the specific gas constant for water vapour, R_{da} is specific gas constant for dry air, and $K_{l_{cd}}^j$ is the permeability with respect to chemical solute. The other parameters were defined before.

Other special features for the bulk air flow and dissolved air are considered. Darcy's law is used for bulk air flow, advection for dissolved air is included and Henry's law for partitioning air between liquid and air phase is used.

2.5.4. Thermal behaviour.

In code COMPASS, the heat transfer process considers conduction, convection and latent heat of vapourisation, as governed by the following equation:

$$C_{Ti} \frac{\partial u_i}{\partial t} + C_{TT} \frac{\partial T}{\partial t} + C_{Ta} \frac{\partial u_a}{\partial t} + C_{Tu} \cdot \frac{\partial \mathbf{u}}{\partial t} = \nabla [K_{Ti} \nabla u_i] + \nabla [K_{TT} \nabla T] + \nabla [K_{Ta} \nabla u_a] + J_T \quad (2.5.33)$$

with

$$C_{Ti} = \left[\begin{array}{l} -\left(C_{pl} \rho_l n - C_{pv} \rho_v n - C_{pda} \rho_{da} n\right) \frac{\partial S_l}{\partial S} - C_{pv} S_a n \left(\rho_0 \frac{\partial h}{\partial S} \right) + \\ C_{pda} S_a n \frac{R_v}{R_{da}} \left(\rho_0 \frac{\partial h}{\partial S} \right) \end{array} \right] (T - T_r)$$

$$+ Ln \rho_v \frac{\partial S_l}{\partial S} - Ln S_a \left(\rho_0 \frac{\partial h}{\partial S} \right)$$

$$C_{TT} = H_c + \left[\begin{array}{l} \left(C_{pl} \rho_l n - C_{pv} \rho_v n - C_{pda} \rho_{da} n\right) \frac{\partial S_l}{\partial T} + C_{pv} S_a n \left(h \frac{\partial \rho_0}{\partial T} + \rho_0 \frac{\partial h}{\partial T} \right) + \\ C_{pda} S_a n \left(-\frac{\rho_{da}}{T} - \frac{R_v}{R_{da}} \left(h \frac{\partial \rho_0}{\partial T} + \rho_0 \frac{\partial h}{\partial T} \right) \right) \end{array} \right] (T - T_r)$$

$$- Ln \rho_v \frac{\partial S_l}{\partial T} + Ln S_a \left(h \frac{\partial \rho_0}{\partial T} + \rho_0 \frac{\partial h}{\partial T} \right)$$

$$C_{Ta} = \left[\begin{array}{l} \left(C_{pl} \rho_l n - C_{pv} \rho_v n - C_{pda} \rho_{da} n\right) \frac{\partial S_l}{\partial S} + C_{pv} S_a n \left(\rho_0 \frac{\partial h}{\partial S} \right) + \\ C_{pda} S_a n \left(\frac{1}{R_{da} T} - \frac{R_v}{R_{da}} \left(\rho_0 \frac{\partial h}{\partial S} \right) \right) \end{array} \right] (T - T_r)$$

$$- Ln \rho_v \frac{\partial S_l}{\partial S} + Ln S_a \left(\rho_0 \frac{\partial h}{\partial S} \right)$$

$$C_{Tu} = \left[\left(-C_{ps} \rho_s + C_{pl} S_l \rho_l + C_{pv} S_a \rho_v + C_{pda} S_a \rho_{da} \right) \mathbf{m}_i^T \mathbf{P} \right] (T - T_r) + LS_a \rho_v \mathbf{m}_i^T \mathbf{P}$$

$$K_{Ti} = -L \rho_l \frac{D_{atms} v_v n}{\rho_l} \left(\rho_0 \frac{\partial h}{\partial S} \right) + (T - T_r) \rho_l \left(C_{pl} k_l \rho_l / \gamma_l - C_{pv} \frac{D_{atms} v_v n}{\rho_l} \left(\rho_0 \frac{\partial h}{\partial S} \right) \right)$$

$$K_{TT} = \lambda_T + L \rho_l \frac{D_{atms} v_v n (\nabla T)_a}{\rho_l \nabla T} \left(h \frac{\partial \rho_0}{\partial T} + \rho_0 \frac{\partial h}{\partial T} \right)$$

$$+ (T - T_r) \rho_l C_{pl} \frac{D_{atms} v_v n (\nabla T)_a}{\rho_l \nabla T} \left(h \frac{\partial \rho_0}{\partial T} + \rho_0 \frac{\partial h}{\partial T} \right)$$



$$K_{Ta} = L\rho_l \frac{D_{atms} \nu_v n}{\rho_l} \left(\rho_0 \frac{\partial h}{\partial S} \right) + L\rho_v k_a$$

$$(T - T_r) \left(\rho_l C_{pv} \frac{D_{atms} \nu_v n}{\rho_l} \left(\rho_0 \frac{\partial h}{\partial S} \right) + \rho_v C_{pv} k_a + \rho_{da} C_{pda} k_a \right)$$

$$J_T = (T - T_r) C_{pl} \rho_l \nabla (k_l \nabla z)$$

where C_{pl} is the specific heat capacity of liquid, C_{pv} is the specific heat capacity of vapour, C_{pda} is the specific heat capacity of dry air, C_{ps} is the heat capacity of solid, T_r is a reference temperature, L is the latent heat of vaporisation, and λ_T is the thermal conductivity of soil, ρ_s is the density of the solid and ρ_{da} is the density of dry air. Other parameters were defined before.

2.5.5. Transport equation.

The mass transport process in the COMPASS code is governed by

$$C_{c_d l}^i \frac{\partial u_l}{\partial t} + C_{c_d a}^i \frac{\partial u_a}{\partial t} + C_{c_d T}^i \frac{\partial T}{\partial t} + C_{c_d c_d}^i \frac{\partial c_d^i}{\partial t} + C_{c_d s}^i \frac{\partial S_s^i}{\partial t} + C_{c_d u}^i \frac{\partial \mathbf{u}}{\partial t} =$$

$$\nabla \cdot [K_{c_d l}^i \nabla u_l] + \nabla \cdot [K_{c_d T}^i \nabla T] + \nabla \cdot [K_{c_d c_d}^i \nabla c_d^i] + \nabla \cdot \left[\sum_{j=1}^{n, (j \neq i)} K_{c_d c_d}^j \nabla c_d^j \right] \quad (2.5.34)$$

$$+ J_{c_d}^i - \lambda_i \theta_l (c_d^i + S_{so}^i)$$

with

$$C_{c_d l}^i = -nc_d^i \frac{\partial S_l}{\partial S}$$

$$C_{c_d a}^i = nc_d^i \frac{\partial S_l}{\partial S}$$

$$C_{c_d T}^i = nc_d^i \frac{\partial S_l}{\partial T}$$

$$C_{c_d c_d}^i = nS_l$$

$$C_{c_d s}^i = nS_l$$

$$C_{c_d u}^i = c_d S_l \mathbf{m}_l^T \mathbf{P}$$

$$K_{c_d l}^i = \frac{c_d^i K_l}{\gamma_l}$$

$$K_{c_d T}^i = \theta_l \tau D^0 S^i$$

$$K_{c_d c_d}^i = n S_l \mathbf{D}_{mn}^i - c_d^i K_l^{c_d^i}$$

$$K_{c_d c_d}^j = -c_d^j K_l^{c_d^j}$$

$$J_{c_d}^i = \nabla \cdot (c_d^i K_l \nabla z)$$

$$\mathbf{D}_{mn}^i = \frac{\alpha_T |v| \delta_{mn}}{\theta_l} + (\alpha_l - \alpha_i) \frac{v_m v_n}{|v| \theta_l} + \tau D^0 \delta_{mn}$$

where \mathbf{D}_{mn}^i , α_l , α_T , τ , δ_{mn} , θ_l , D^0 , $|v|$, v_m and v_n represents hydrodynamic dispersion (tensor), longitudinal dispersivity, lateral dispersivity, tortousity, Kronecker delta (=1 if $m = n$, otherwise =0), volumetric liquid content, free solution diffusion coefficient, average liquid velocity and liquid velocities.

Parameter s_s^i is the sink/source term and represents change in concentration due to adsorption, desorption, precipitation, dissolution and redox transformations as appropriate. This term is evaluated through the geochemical model.

Optionally, a radioactive term is added to the RHS of equation (5.33), where s_{so}^i and λ_i represent the sorbed (adsorbed + precipitated, as appropriate) concentration of chemical component i and radioactive decay coefficient of the i^{th} component, respectively, and s_{so}^i is the secondary variable and hence not solved directly.

In the COMPASS code, some special features for transport processes are also considered, such as reactive and non-reactive transport, diffusion, mechanical dispersion, thermal diffusion, advection, and the sink/source terms linking the geochemical model, MINTEQA2.

In the COMPASS code, some special features for transport processes are also considered, such as reactive and non-reactive transport, diffusion, mechanical dispersion, thermal diffusion, advection, and the sink/source terms linking the geochemical model, MINTEQA2. The radioactive decay is included in the sink/source terms.



2.5.6. Geochemical processes.

For WP4 of the THERESA project, the geochemical processes are represented by two governing equations: a mass action equation and a mass balance equation.

The mass action equation is written

$$K_{mi} = [C_{mi}] \prod X_j^{a_{mi,j}} \quad (2.5.35)$$

and the mass balance equation is given by

$$Y_j = \sum a_{mi,j} C_{mi} - M_j \quad (2.5.36)$$

where K_{mi} is the equilibrium constant for the formation of species mi , C_{mi} is the concentration of species mi , $[C_{mi}]$ is the activity of species mi , X_j is the activity of component j , $a_{mi,j}$ is the stoichiometric coefficient of component j in species mi , \prod denotes the product over all components in species mi , and $mi = 1 \dots m$, M_j is the total dissolved concentration of component j (also referred to as the total analytical concentration) and is the known (or measured) input, Y_j is the difference between the calculated total dissolved concentration of component j and the known analytical total dissolved concentration of component j .

The geochemical model in the COMPASS code is based on equilibrium geochemistry as implemented in MINTEQA2. The model is capable of computing equilibrium among the dissolved (speciation, complexation, acid-base, redox), adsorbed (linear isotherm, nonlinear isotherm, ion exchange, electrostatic models), solid (mineral precipitation and/or dissolution) and gas phases (fixed partial pressure), and incorporates an extensive thermodynamic database.

2.6. IRSN (CAST3M)

CAST3M is a finite element code developed by CEA and used by IRSN. The hydro-mechanical formulation is solved in a coupled manner, but the thermal behaviour dominated by heat conduction is considered uncoupled.

2.6.1. Mathematical formulation.

The code solves simultaneously the following fundamental balance equations:

- Mass balance of water (liquid and vapour):

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$$\frac{\partial m_w}{\partial t} + \nabla \cdot (W_l + W_v) = 0 \quad (2.6.1)$$

- Internal energy balance for the medium:

$$\rho c(S_l) \frac{\partial T}{\partial t} = \nabla \cdot (\lambda(S_l) \nabla T) \quad (2.6.2)$$

- Momentum balance of the medium:

$$\nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{F} = \mathbf{0} \quad (2.6.3)$$

where: m_w : mass of water, W_l : mass flux of liquid water, W_v : mass flux of vapour,
 $\rho c(S_l)$: heat capacity depends on saturation degree. $\rho c(S_l) = \phi S_l \rho_l c_l + (1 - \phi) \rho_s c_s$
 ρ : is the equivalent density. $\rho = (1 - \phi) \rho_s + \phi S_l \rho_l$

2.6.2. Mechanical constitutive law.

$$d\boldsymbol{\sigma} = \mathbf{C}(d\varepsilon - \alpha d\mathbf{T}) - \mathbf{B} dp_l \quad (2.6.4)$$

where \mathbf{C} is the elastic tensor, \mathbf{B} is the Biot's coefficient tensor which in unsaturated case is assumed dependant on the capillary pressure:

$$\mathbf{B} = b(p_c) \mathbf{I} \quad (2.6.5)$$

where:

$$b(p_c) = \frac{P_{ref}}{P_{ref} + p_c}$$

$$P_{ref} = \ln p_s$$

$$\ln p_s = 6.77 \rho_d - 9.07$$

p_s is the swelling pressure

2.6.3. Hydraulic constitutive law.

The mass flux of liquid water is given by the generalized Darcy's law:

$$W_l = -\frac{K_w}{\eta_l(T)} k_{rl}(S_l) \nabla p_l \quad (2.6.6)$$

where: K_w : is the intrinsic permeability, k_{rl} : is the relative permeability, η_l : is the dynamic viscosity of water

The intrinsic permeability of the bentonite depends on its dry density:

$$\log K_w = -2.96\rho_d - 8.57$$

The relative permeability is calculated by:

$$k_{rl}(S_l) = S_l^3$$

The mass flux of vapour is due to diffusion (constant gas pressure):

$$W_v = -\frac{M_v}{RT} \phi S_g \tau D_{va} \nabla p_v \quad (2.6.7)$$

where M_v is the mola mass of vapour, R is the ideal gas constant, $S_g = 1 - S_l$, τ is the tortuosity, D_{va} is the diffusion of vapour in air.

$$D_{va} = 0.217 \frac{P_{atm}}{P_g} \left(\frac{T}{T_o} \right)^{1.88}$$

The vapour pressure is calculated using Kelvin's law:

$$p_v = p_{vs}(T) \exp\left(-\frac{p_c M_v}{\rho_l R}\right) \quad (2.6.8)$$

where $p_{vs}(T)$ is the saturated vapour pressure which depends on temperature.

Thus, the mass flux of vapour can be express as:

$$W_v = -D_{vT} \nabla T - D_{vp} \nabla p_l \quad (2.6.9)$$

Finally, the gravimetric water content w is related to the capillary pressure by the following retention curve:

$$\omega = (a + b\phi) \left[1 + \left(\frac{p_c}{p_0 \exp(-\eta(\phi - \phi_0)) \exp(-\alpha(T - T_0))} \right)^{\frac{1}{1-\lambda}} \right]^{-\lambda} \quad (2.6.10)$$

2.6.4. Thermal constitutive law

The thermal conductivity is calculated by:

$$\lambda = \frac{A_1 + A_2}{1 + \exp\left(\frac{S_l - x_0}{dx}\right)} + A_2 \quad (2.6.11)$$



3. Code Improvements.

In the following section the improvements of codes proposed by the different teams are described. The descriptions are based on the corresponding reports submitted by the various teams.

3.1. CIMNE (Code_Bright).

The main improvement proposed for Code_Bright consists in the implementation of interface elements. The formulation should allow the simulation of the coupled hydro-mechanical behaviour of interfaces. The mathematical formulation and the constitutive law for the interface element are presented below:

3.1.a. Mathematical formulation

- **Elasto- viscoplastic model for discontinuities.**

An elasto-viscoplastic model was implemented into CODE_BRIGHT because this formulation allows the treatment of non-associated plasticity and strain softening behaviour of materials. Moreover, using the viscoplasticity it is possible considered the variation of the strain rate with time. The concept of viscoplasticity is based on the development done by Perzyna (1963), Zienkiewicz et al. (1974), Lorefice et al.(2007).

The total strain $\boldsymbol{\varepsilon}$ is calculated by addition of reversible elastic strain, $\boldsymbol{\varepsilon}^e$, and viscoplastic strain $\boldsymbol{\varepsilon}^{vp}$, which are zero when stresses are below a threshold value (the yield surface):

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^e + \boldsymbol{\varepsilon}^{vp} \quad (3.1.1)$$

All strains are represented by a vector of three quantities in two-dimensional case and have the following components:

$$\boldsymbol{\varepsilon}^T = \left[\varepsilon_{xx}, \varepsilon_{yy}, \gamma_{xy} \right] \quad (3.1.2)$$

The elastic behaviour of the interface always is studied related the normal effective ($\sigma'n$) and the tangential stresses (τ) with the normal (u_n) and the tangential (u_s) displacement of the interface element respectively, using the normal and the tangential stiffness (eq.3.1.3). The normal stiffness depends on the aperture of the discontinuity as it is shown in eq. 3.1.3.

$$\begin{Bmatrix} \sigma'_n \\ \tau \end{Bmatrix} = \begin{bmatrix} k_n & 0 \\ 0 & k_s \end{bmatrix} \begin{Bmatrix} u_n \\ u_s \end{Bmatrix} \quad k_n = \frac{m}{a - a_{\min}} \quad (3.1.3)$$

The local strains are calculated dividing the normal and the tangential displacement of the interface respect to its initial aperture (a) (eq.3.1.3).

$$\begin{Bmatrix} u_n / a_0 \\ u_s / a_0 \end{Bmatrix} = 1/a_0 \begin{bmatrix} 1/k_n & 0 \\ 0 & 1/k_s \end{bmatrix} \begin{Bmatrix} \sigma'_n \\ \tau \end{Bmatrix} \quad (3.1.4)$$

$$\begin{Bmatrix} \varepsilon_n \\ \gamma \end{Bmatrix} = 1/a_0 \begin{bmatrix} 1/k_n & 0 \\ 0 & 1/k_s \end{bmatrix} \begin{Bmatrix} \sigma'_n \\ \tau \end{Bmatrix}$$

Then, these strains are rotated to the global system of coordinates (eq.3.1.5).

$$\begin{Bmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \gamma_{xy} \end{Bmatrix} = \mathbf{T}^T(\phi) \begin{bmatrix} 1/k_n a_0 & 0 & 0 \\ 0 & 1/E & 0 \\ 0 & 0 & 1/k_s a_0 \end{bmatrix} \mathbf{T}(\phi) \begin{Bmatrix} \sigma'_x \\ \sigma'_y \\ \tau_{xy} \end{Bmatrix} \quad (3.1.5)$$

The viscoplastic displacements are calculated by:

$$\frac{d}{dt} \mathbf{u}^{vp} = \gamma \langle \phi(F) \rangle \frac{\partial Q}{\partial \boldsymbol{\sigma}} \quad (3.1.6)$$

where: γ is a fluidity parameter. To ensure no viscoplastic flow below the yield it is imposed that:

$$\begin{aligned} \langle \phi(F) \rangle &= 0 & \text{if } F < 0 \\ \langle \phi(F) \rangle &= \phi(F) & \text{if } F \geq 0 \end{aligned} \quad (3.1.7)$$

Then the visco-plastic displacement rate is given by a power of law for Φ ,

$$\begin{aligned} \Delta u_n^{vp} &= \gamma F^N \frac{\partial Q}{\partial \sigma} \Delta t \\ \Delta u_s^{vp} &= \gamma F^N \frac{\partial Q}{\partial \tau} \Delta t \end{aligned} \quad (3.1.8)$$

And the displacements are related with the stress state by the tangent viscoplastic consistent matrix (compliance matrix), which is calculated by:

$$C^{vp} = T(\phi)^T \begin{bmatrix} \frac{\partial \Delta u_n^{vp}}{\partial \sigma} & 0 & \frac{\partial \Delta u_n^{vp}}{\partial \tau} \\ 0 & 0 & 0 \\ \frac{\partial \Delta u_s^{vp}}{\partial \sigma} & 0 & \frac{\partial \Delta u_s^{vp}}{\partial \tau} \end{bmatrix} T(\phi)$$

$$\begin{aligned} \frac{\partial \Delta u_n^{vp}}{\partial \sigma} &= \gamma N F^{N-1} f_\sigma^{dil} f_c^{dil} \left[2tg\phi(c - \sigma'tg\phi) \right]^2 \Delta t + \\ &+ \gamma F^N \left[-2tg\phi f_c^{dil} \frac{|\sigma'|}{\sigma^{dil}} (c - \sigma'tg\phi) - 2tg^2\phi f_\sigma^{dil} f_c^{dil} \right] \Delta t \end{aligned} \quad (3.1.9)$$

$$\frac{\partial \Delta u_n^{vp}}{\partial \tau} = \gamma N F^{N-1} 2\tau f_\sigma^{dil} f_c^{dil} \left[2tg\phi(c - \sigma'tg\phi) \right] \Delta t$$

$$\frac{\partial \Delta u_s^{vp}}{\partial \sigma} = \gamma N F^{N-1} 2\tau \left[2tg\phi(c - \sigma'tg\phi) \right] \Delta t$$

$$\frac{\partial \Delta u_s^{vp}}{\partial \tau} = \gamma N F^{N-1} 2\tau \Delta t + \gamma F^N 2\Delta t$$

3.1.b. Mechanical constitutive law.

The elastic tangential stiffness is assumed to be constant, whereas the value of the normal elastic stiffness depends on the loading conditions and the interface aperture as:

$$\sigma = m \frac{u^e}{u_{mc} - u^e} \quad (3.1.10)$$

To calculate the visco-plastic strains of the interface, it is necessary to define a yield surface F and a plastic potential Q as well as a dilatancy law. A yield condition based on fracture mechanics is adopted (Carol et al., 1997):

$$F \equiv \sigma_T^2 - (c - \sigma_N \tan \phi)^2 + (c - \chi \tan \phi)^2 \quad (3.1.11)$$

where $\tan\Phi$, c , and χ are model parameters representing the slope, the cohesion of the asymptote and the tensile strength of the interface respectively. This curve will result in a smooth transition between two limit states: Mode I and Mode IIa loading conditions. Softening laws: The shrinkage of the cracking surface for both modes is achieved with the evolution of the parameters $\tan\Phi$, c , and χ as a function of the work spent on fracture processes during formation of the crack.

$$dW^{cr} = \sigma_N du_N^{cr} - \sigma_T du_T^{cr} \quad \sigma_N \geq 0 \quad (\text{tension})$$

$$dW^{cr} = \sigma_T du_T^{cr} \left(1 - \left| \frac{\sigma_N \tan \phi}{\sigma_T} \right| \right) \quad \sigma_N < 0 \quad (\text{compression}) \quad (3.1.12)$$

where dW^{cr} is the increment of work spent on fracture processes and du_N^{cr} du_T^{cr} are the increment of the normal and tangential displacement of the crack respectively.

The variation of $\tan\Phi$, c , and χ is assumed to be linear in terms of the intermediate scaling function f , defined as:

$$f(\xi) = \frac{\xi e^{-\alpha}}{1 + (e^{-\alpha} - 1)\xi}$$

$$\xi = \frac{W^{cr}}{G_f^I} \quad ; \quad \alpha = \alpha_\chi \quad (3.1.13)$$

$$\xi = \frac{W^{cr}}{G_f^{IIa}} \quad ; \quad \alpha = \alpha_\phi \quad ; \quad \alpha = \alpha_c$$

where G_f^I is the fracture energy dissipated by Mode I and G_f^{IIa} is the fracture energy dissipated by Mode IIa of fracture; the values of the α defined the different evolution of the parameters Φ , c , and χ like it is shown in Figure 13 b and c.

Plastic potential surface and dilatancy: Initially, the potential surface coincides with the cracking surface in tension, while in compression the rule is non associated, with dilatancy vanishing for compression intensity approaching the value σ^{dil} (compression strength of the material), which is an additional parameter of the model. The amount of dilatancy must also decrease with increasing degradation of the crack surface, so that it vanishes completely for the residual friction state given by $c = 0$. The following expressions describe all these effects:

$$\frac{\partial Q}{\partial \sigma_N} = 2 \tan \phi (c - \sigma_N \tan \phi) f_\sigma^{dil} f_c^{dil} \quad ; \quad \frac{\partial Q}{\partial \sigma_T} = 2 \sigma_T \quad (3.1.14)$$

where f_σ^{dil} and f_c^{dil} are calculated by:

$$f(\xi) = \frac{\xi e^{-\alpha}}{1 + (e^{-\alpha} - 1)\xi}$$

$$\xi = \frac{|\sigma_N|}{\sigma^{dil}} \quad ; \quad \alpha = \alpha_{\sigma}^{dil} \quad (3.1.15)$$

$$\xi = \frac{c}{c_0} \quad ; \quad \alpha = \alpha_c^{dil}$$

3.1.c. Hydraulic constitutive law.

The flux flow through the discontinuity will be calculated with the Darcy's law (equation 3.1.16). The longitudinal and transversal intrinsic permeability of the interface will be considered. And the real distribution of pressure along the discontinuity axis is approximated through interpolation of the nodal values of the zero thickness interface element.

$$\mathbf{q}_{\alpha} = -\frac{\mathbf{k}k_{r\alpha}}{\mu_{\alpha}}(\nabla P_{\alpha} - \rho_{\alpha}\mathbf{g})$$

$$\begin{pmatrix} q_l \\ q_t \end{pmatrix} = \begin{bmatrix} k_{ll} & 0 \\ 0 & k_{tt} \end{bmatrix} \begin{bmatrix} \frac{\partial P}{\partial l} \\ \frac{\partial P}{\partial t} \end{bmatrix} \quad (3.1.16)$$

where \mathbf{q}_{α} is the flux vector along porous media, \mathbf{k} is the intrinsic permeability tensor, $k_{r\alpha}$ is the phase relative permeability, μ_{α} is the viscosity of the fluid, P_{α} is the pressure of the fluid, and ρ_{α} is the density of the fluid. Gravity is represented by the vector \mathbf{g} . The longitudinal transmissibility of the discontinuity depends on its normal aperture and roughness calculated using the following expression (Barton's Law):

$$k_{ll} = \frac{a^2}{JRC^{2.5}12} \quad (3.1.17)$$

The transversal permeability k_{tt} is considered equal to the transversal permeability of the continuum media.

3.2. Posiva/Marintel (FreeFEM++).

The improvement proposed is a thermodynamic approach to modelling of re-saturation of bentonite buffer. The model is based on assumption that Helmholtz energy can be divided into shear energy, swelling energy and hydration energy. The mathematical formulation is described below:

3.2.1. Mechanical behaviour.

$$\sigma = \frac{\partial \psi_{HM}}{\partial \varepsilon} \quad (3.2.1)$$

$$\sigma_{ij}^D = \frac{\partial \psi_{HM}}{\partial \varepsilon_{ij}^D} \quad (3.2.3)$$

$$\psi_{HM} = \frac{1}{2} P_{sw}(\varepsilon) \left(\varepsilon - \frac{m^w}{\rho_\alpha^w} + \phi_R \right)^2, \text{ when } \frac{m^w}{\rho_\alpha^w} - \varepsilon > \phi_R \text{ and } \frac{m^w}{\rho_\alpha^w} > \phi_{sw} \quad (3.2.4)$$

$$\psi_{HM} = \frac{1}{2} P_{sw}(0) \left(\varepsilon - \frac{m^w}{\rho_\alpha^w} + \phi_R \right)^2, \text{ when } \phi_R \geq \frac{m^w}{\rho_\alpha^w} - \varepsilon \text{ and } \frac{m^w}{\rho_\alpha^w} > \phi_{sw} \quad (3.2.5)$$

$$\psi_{HM} = \frac{1}{2} P_{sw}(0) (\varepsilon - \phi_{sw} + \phi_R)^2, \text{ when } \frac{m^w}{\rho_\alpha^w} \leq \phi_{sw} \quad (3.2.6)$$

$$P_{sw}(\varepsilon) = S_{CL} [\rho^w(\phi_0 + \varepsilon)] / (\phi_0 - \phi_R) \quad (3.2.7)$$

$$\psi_S = G \varepsilon_{ij}^D : \varepsilon_{ij}^D \quad (3.2.8)$$

$$G = \frac{3(1-2\nu)}{2(1+\nu)} K^o \quad (3.2.9)$$

$$K^o = \frac{\partial^2 \psi_{HM}}{\partial \varepsilon^2} - \left(\frac{\partial^2 \psi_{HM}}{\partial \varepsilon \partial m^w} \right)^2 \left(\frac{\partial^2 (\psi_{HM} + \psi_M)}{(\partial m^w)^2} \right)^{-1} \quad (3.2.10)$$

where σ is the average normal total stress, $\sigma = \sigma_{ii}/3$, σ_{ij}^D the deviatoric stress tensor, $\sigma_{ij}^D = \sigma_{ij} - \sigma \delta_{ij}$, where δ_{ij} is the Kronecker delta; ε is the dilation (volume strain) $\varepsilon = \varepsilon_{ii}$; ε_{ij}^D is the deviatoric strain tensor, $\varepsilon_{ij}^D = \varepsilon_{ij} - \varepsilon \delta_{ij} / 3$; ψ_{HM} is the hydro-mechanical part of the Helmholtz energy density; m^w is the water mass content (all

phases); ρ^w is the density of liquid water (model parameter); γ_{sw} is the swelling factor; P_{sw} is the swelling function; $S_{CL}(m^w)$ is the unconfined suction curve; ϕ_0 is the initial porosity, $\rho_s(1-\phi_0)=\rho_{d0}$; ρ_{d0} is the initial dry density; ϕ_R is the volume fraction of high swelling, $\phi_R = \phi_0$; ϕ_{sw} is the volume fraction of no swelling, $\phi_{sw}=0.07\rho_{d0}/\rho^w$; ψ_S is the shear-related part of the Helmholtz energy density; G is the shear modulus; ν is the Poisson ratio; and K^o is the dry bulk modulus.

3.2.2. Hydraulic behaviour.

The fluid flow equation is viewed as moisture diffusion governed by

$$\frac{dm^w}{dt} + \frac{\partial}{\partial x_i} \left(D_\varepsilon \frac{\partial}{\partial x_i} \varepsilon - D_m \frac{\partial}{\partial x_i} m^w - D_T \frac{\partial}{\partial x_i} T + \sum_\alpha J_\alpha^w \right) = 0 \quad (3.2.11)$$

where

$$K_{sat}^* = K_r^* 10^{-\kappa_w \frac{\rho_{d0}}{\rho^w} - \kappa_0} \quad (3.2.12)$$

$$D_m = \rho^w \frac{K_{sat}^*}{g} (S_r)^\delta \frac{\partial^2 (\psi_{HM} + \psi_H)}{(\partial m^w)^2} \quad (3.2.13)$$

$$D_\varepsilon = \rho^w \frac{K_{sat}^*}{g} (S_r)^\delta \frac{\partial^2 \psi_{HM}}{\partial m^w \partial \varepsilon} \quad (3.2.14)$$

$$D_T = \tau_T (S_r) D_m \quad (3.2.15)$$

with

$$S_r = m^w / [\rho^w (\phi_0 + \varepsilon)] \quad (3.2.16)$$

$$\frac{\partial \psi_H}{\partial m^w} = -\frac{1}{\rho^w} S_{CL}(m^w) \quad (3.2.17)$$

where D_m is the moisture diffusion coefficient, D_ε is the dilational moisture diffusion coefficient, D_T is the thermal moisture diffusion coefficient, T the temperature, J_α^w is the osmotic flow caused by concentration gradient of solute species α , K_{sat}^* is the hydraulic conductivity of water saturated material, K_r^* is the scaling parameter of hydraulic conductivity, $K_r^* = 1.0$ m/s, κ_w is the initial density exponent of hydraulic conductivity, κ_0 is the exponent of hydraulic conductivity, g is the gravitational acceleration, S_r is the degree of saturation, δ is the relative conductivity exponent, ψ_H

is the hydraulic part of the Helmholtz energy density, and $\tau_T(S_r)$ is the vapour flow function.

Retention curve

The expression used here for unconfined suction curve for compacted bentonite is

$$\log(s/s_0) = -\left(a \frac{\rho_{d0}}{\rho^w} - b\right)^{-1} \left[\frac{m^w}{\rho_{d0}} - \left(c \frac{\rho_{d0}}{\rho^w} - d\right) \right] \quad (3.2.18)$$

where a , b , c and d are empirical constants, and $s_0 = 1.0$ MPa is a dimensioning parameter.

The vapour flow function, which relates empirically the vapour permeability to hydraulic conductivity, is assumed to be

$$\tau_T(S_r) = 0, \text{ for } S_r \leq 0.15 \text{ or } S_r \geq 0.95 \quad (3.2.19)$$

$$\tau_T(S_r) = \tau_R, \text{ for } 0.6 \leq S_r \leq 0.8 \quad (3.2.20)$$

$$\tau_T(S_r) = \tau_R \frac{S_r - 0.2}{0.4}, \text{ for } 0.2 \leq S_r \leq 0.6 \quad (3.2.21)$$

$$\tau_T(S_r) = \tau_R \frac{0.95 - S_r}{0.15}, \text{ for } 0.8 \leq S_r \leq 0.95 \quad (3.2.22)$$

where τ_R is the intermediate value of vapour flow function (model parameter).

Diffusive flux J_ζ (Na^+ + Cl^-)

$$J_\alpha = -D_\alpha \frac{\partial}{\partial x_i} c_\alpha \quad (3.2.23)$$

$$-D_{\alpha T} \frac{\partial}{\partial x_i} T \quad (3.2.24)$$

3.2.3. Chemical behaviour.

The chemical processes considered are chemical equilibrium and chemical species transport processes. The equations for chemical equilibrium and transport of species given below are preliminary equations that will be modified according to the water

chemistry transport processes to be simulated. There are also alternative ways to solve these equations, depending on the type of chemical processes.

The chemical equilibrium is governed by

$$\Delta_r G_{mL}^0 = -RT \ln K_L \quad (3.2.25)$$

where

$$K_L = \prod_{(\alpha,K) \in L} (a_K^\alpha)_{eq}^{v_{KL}^\alpha} \quad (3.2.26)$$

and the transport of species is governed by

$$\sum_{(\alpha,K) \in L} \left(\frac{\partial m_K^\alpha}{\partial t} + \frac{\partial}{\partial x_i} w_K^\alpha \right) = 0 \quad (3.2.27)$$

$$w_i^{K\alpha} = m_K^\alpha U_i^K + J_i^{K\alpha} \quad (3.2.28)$$

$$J_i^{K\alpha} = \phi_K D_K^\alpha \frac{\partial}{\partial x_i} \mu^\alpha \quad (3.2.29)$$

$$\frac{\partial \psi}{\partial m_K^\alpha} = \frac{\mu^\alpha}{\omega^\alpha} \quad (3.2.30)$$

where $\Delta_r G_{mL}^0$ is the standard molar Gibbs energy of reaction, a model parameter, K_L the thermodynamic equilibrium constant of reaction L , $(a_K^\alpha)_{eq}$ is the activity of species α in phase K in equilibrium (formula depends on the type of reaction), v_{KL}^α is the stoichiometric coefficient of species α in phase K in reaction L , m_K^α is the mass content of species α in phase K , $w_i^{K\alpha}$ is the mass flux of species α in phase K , U_i^K is the volume flux (average velocity) of phase K , $J_i^{K\alpha}$ is the diffusive flux of species α in phase K , ϕ_K is the volume fraction of phase K , D_K^α is the diffusion coefficient of species α in phase K , ψ is the total Helmholtz energy density, μ^α is the chemical potential of species α (formula depends on the type of reaction), and ω_K^α is the molar mass of species α .

3.3. KTH (ROLG).

Several improvements will be implemented by KTH in the ROLG code. The new formulation will include the effects of deformation, gas pressure, liquid pressure, temperature and swelling deformations in the mechanical behaviour. For fluid flow temperature, gas, phase change, thermo-osmosis and porosity changes are considered. Also gas phase and vapour diffusion are included in the code. The mathematical formulation of the improvements is presented below:

3.2.4. Mechanical behaviour.

The equilibrium equation of the bentonite includes the effects of deformation, gas pressure, liquid pressure, temperature and water induced swelling deformation process, governed by

$$\nabla \cdot (\mathbf{D} : \frac{\partial \boldsymbol{\varepsilon}}{\partial t}) - \nabla \cdot [I(1-\chi) \frac{\partial p_g}{\partial t} - \nabla \cdot (I\chi \frac{\partial p_l}{\partial t})] - \nabla \cdot [\mathbf{D} : (I\beta \frac{\partial T}{\partial t})] - \nabla \cdot (\mathbf{D} : \frac{\partial \boldsymbol{\varepsilon}'}{\partial t}) + \frac{\partial \mathbf{F}}{\partial t} = 0 \quad (3.3.1)$$

where $\boldsymbol{\varepsilon}$ is the total strain tensor, I the identity tensor, χ the effective stress parameter or Bishop's parameter, p_l the liquid pressure, p_g the gas pressure, T the temperature, β the thermal linear expansion coefficient of skeleton, and \mathbf{F} the body force vector. \mathbf{D} is the elasticity tensor or elastoplastic tensor depending on the constitutive model of material. $\boldsymbol{\varepsilon}'$ is the swelling strain which is a function of volumetric water content.

3.2.5. Hydraulic behaviour.

The equation of fluid flow considers the effects of temperature, gas pressure, liquid pressure, volume deformation, phase change, thermo-osmosis and the effect of porosity change, governed by

$$C_T^l \frac{\partial T}{\partial t} + C_g^l \frac{\partial p_g}{\partial t} + C_l^l \frac{\partial p_l}{\partial t} + \frac{\partial \varepsilon_b}{\partial t} + S_{re} \frac{\partial n}{\partial t} - \nabla \cdot [\frac{k_r^l k}{\mu_l} (\nabla p_l + \rho_l \mathbf{g})] - \nabla \cdot (k_T^l \nabla T) + \frac{1}{\rho_l} q_p = 0 \quad (3.3.2)$$

where k is the intrinsic permeability, μ_l is the fluid viscosity, k_r^l the liquid relative permeability, ε_b the bulk strain, \mathbf{g} the gravitational acceleration vector, k_T^l is the coefficient of thermal coupling for liquid flux. The other coefficients are defined as follows

$$S_{re} = \frac{\rho_l(1+H)S_r - \rho_v}{\rho_l - \rho_v}$$

$$C_g^l = \frac{n \partial S_{re}}{\partial (p_g - p_l)} \equiv \frac{n \partial S_{re}}{\partial s}$$



$$C_l^l = \frac{nS_{re}}{\rho_l} \frac{\partial \rho_l}{\partial p_l} - \frac{n\partial S_{re}}{\partial s} = \frac{nS_{re}}{K_l} - \frac{n\partial S_{re}}{\partial s}$$

$$C_T^l = \frac{nS_{re}}{\rho_l} \frac{\partial \rho_l}{\partial T} = -nS_{re}\beta_l$$

where, S_r is the saturated degree, H the coefficient of solubility of gas in liquid, ρ_g the gas density, ρ_l the liquid density, ρ_v the vapor density, n the porosity, s the suction. Moreover, q_p is the phase change part which can be described using Dalton's equation

$$q_p = \rho_l \omega (p_{sv} - p_v) \quad (3.3.3)$$

where $\omega > 0$ is liquid phase transfer coefficient, p_v is the vapour pressure, and p_{sv} is the saturated vapour pressure.

3.2.6. Gas flow equation-the gas phase transport process

The mixture of air and water vapour is treated as a homogenous gas. The equation of gas flow considers the effects of temperature, gas pressure, liquid pressure, volume deformation, phase change, thermo-osmosis and the effect of porosity change, described by

$$C_T^g \frac{\partial T}{\partial t} + C_g^g \frac{\partial p_g}{\partial t} + C_l^g \frac{\partial p_l}{\partial t} + \frac{\partial \varepsilon_b}{\partial t} + (1 - S_{re}) \frac{\partial n}{\partial t} - \nabla \cdot \left[\frac{k_r^g k}{\mu_g} (\nabla p_g + \rho_g \mathbf{g}) \right] - \nabla \cdot [k_T^g \cdot \nabla T] - \frac{1}{\rho_g} q_p = 0 \quad (3.3.4)$$

where μ_g is the fluid viscosity, k_r^g the liquid relative permeability, k_T^g is the coefficient of thermal coupling for gas flux. The main coefficients are defined as follows

$$C_T^g = \frac{n(1 - S_{re})}{\rho_g} \frac{\partial \rho_g}{\partial T} = -\frac{n(1 - S_{re})}{T}$$

$$C_g^g = \frac{n(1 - S_{re})}{\rho_g} \frac{\partial \rho_g}{\partial p_g} - \frac{n\partial S_{re}}{\partial s} = \frac{n(1 - S_{re})}{p_g} - \frac{n\partial S_{re}}{\partial s}$$

$$C_l^g = \frac{n\partial S_{re}}{\partial s}$$

3.2.7. Vapour flow equation.

The vapour transport includes the diffusion due to vapour gradient and advection due to the movement of gas. Thus, the equation of vapour flow can be expressed by

$$\begin{aligned}
C_T \frac{\partial T}{\partial t} + C_v \frac{\partial p_v}{\partial t} + C_g \frac{\partial p_g}{\partial t} + C_l \frac{\partial p_l}{\partial t} + \frac{\partial \varepsilon_b}{\partial t} + (1 - S_{re}) \frac{\partial n}{\partial t} - \nabla \cdot \left[\frac{k_r^g k}{\mu_g} (\nabla p_g + \rho_g \mathbf{g}) \right] \\
- \nabla \cdot [k_i^g \cdot \nabla T] - \nabla \cdot (D_{ve} \cdot \nabla p_v) - \frac{1}{\rho_v} q_p = 0
\end{aligned} \tag{3.3.5}$$

The main coefficients are defined as follows

$$\begin{aligned}
C_T^v &= \frac{n(1 - S_{re})}{\rho_v} \frac{\partial \rho_v}{\partial T} = -\frac{n(1 - S_{re})}{T} \\
C_v^v &= \frac{n(1 - S_{re})}{\rho_v} \frac{\partial \rho_v}{\partial p_v} = \frac{n(1 - S_{re})}{p_v} \\
C_g^v &= -\frac{n \partial S_{re}}{\partial S} \\
C_l^v &= \frac{n \partial S_{re}}{\partial S} \\
D_{ve} &= D_v \frac{1}{\rho_w RT} = \frac{D_v}{T} \times 2.165 \times 10^{-6}
\end{aligned}$$

where, D_v is the molecular diffusivity of vapour in pore gas. The other parameters were defined previously.

3.2.8. Solid mass conservation equation.

The flow equations above are mass conservation equations of liquid, gas and vapour respectively. In order to maintain consistency of three phases (solid, liquid and gas), the computation of the porosity is required. According to the conservation of solid mass, the equation of porosity can be obtained as follows

$$\begin{aligned}
\frac{1}{\rho_s} \left[\frac{\partial \rho_s}{\partial T} \frac{\partial T}{\partial t} + \chi \frac{\partial \rho_s}{\partial p_l} \frac{\partial p_l}{\partial t} + (1 - \chi) \frac{\partial \rho_s}{\partial p_g} \frac{\partial p_g}{\partial t} + \frac{\partial \rho_s}{\partial \sigma} \left(K \frac{\partial \varepsilon_b}{\partial t} - 3K\beta \frac{\partial T}{\partial t} - \chi \frac{\partial p_l}{\partial t} - (1 - \chi) \frac{\partial p_g}{\partial t} \right) \right] \\
+ \frac{\partial \ln(1 - n)}{\partial t} + \frac{\partial \varepsilon_b}{\partial t} + \frac{\partial u_i}{\partial t} \frac{\partial (\ln(1 - n))}{\partial x_i} = 0
\end{aligned} \tag{3.3.6}$$

where, K is the bulk modulus of skeleton, σ_v the effective confining pressure. The other parameters were defined previously.

3.2.9. Thermal constitutive law.

The heat conduction and convection processes are considered in the code ROLG, but not heat radiation. The effect of the mechanical deformation is also included. The process is governed by the equation

$$C_c^T \frac{\partial T}{\partial t} - \nabla \cdot (C_T^T \nabla T) - \nabla \cdot [C_g^T (\nabla p_g + \rho_g \mathbf{g})] - \nabla \cdot [C_l^T (\nabla p_l + \rho_l \mathbf{g})] + C_s^T \frac{\partial \varepsilon_b}{\partial t} - Q = 0 \quad (3.3.7)$$

where, Q is the heat resource, and other coefficient are defined as follows

$$C_c^T = (1-n)\rho_s c_s + nS_{re}\rho_l c_l + n(1-S_{re})\rho_g c_g$$

$$C_T^T = k_T + \rho_l c_l T k_T^l + \rho_g c_g T k_T^g + K_l \beta_l (T - T_0) \frac{1}{nS_{re}} k_T^l + K_g \beta_g (T - T_0) \frac{1}{n(1-S_{re})} k_T^g$$

$$C_g^T = \rho_g c_g T \frac{k_r^g k}{\mu_g} + K_g \beta_g (T - T_0) \frac{1}{n(1-S_{re})} \frac{k_r^g k}{\mu_g}$$

$$C_l^T = \rho_l c_l T \frac{k_r^l k}{\mu_l} + K_l \beta_l (T - T_0) \frac{1}{nS_{re}} \frac{k_r^l k}{\mu_l}$$

$$C_s^T = [(1-n)\rho_s c_s + \rho_l c_l + \rho_g c_g] T + 3K\beta(T - T_0) + K_l \beta_l (T - T_0) \frac{1}{nS_{re}} + K_g \beta_g (T - T_0) \frac{1}{n(1-S_{re})}$$

where, k_T the thermal conductivity, T_0 the absolute zero temperature ($=-273^\circ\text{C}$), c_s , c_l , c_g are the specific heat capacity of solid, liquid and gas phase respectively, K_l and K_g are the bulk modulus of liquid phase and gas phase respectively, β_l the thermo expansion coefficient of liquid phase, β_g the thermo expansion coefficient of gas phase. The other parameters were defined previously.

3.4. Quintessa (QPAC-EBS).

The improvements proposed by Quintessa are aimed to incorporate processes that are important for bentonite to be properly represented: the inclusion of bentonite swelling and the binding of water to minerals.

3.4.1. Swelling pressure

Swelling of the bentonite is represented through the addition or removal of elastic strain according to the defined swell pressure, consistent with the above relations. The swelling pressure under saturation is defined by:

$$\sigma_{swell} = \sigma_{sat} S_\sigma \left(\frac{S_w - S_{w_{init}}}{1 - S_{w_{init}}} \right) \quad (3.4.1)$$

where σ_{swell} is the swelling pressure at a given saturation (Pa), σ_{sat} is the saturated swell pressure (Pa), S_σ is an empirically derived function relating the relative change in saturation from initial conditions to full saturation (-), S_w is the total water saturation (-), $S_{w_{init}}$ is the initial water saturation (-), respectively.

3.4.2. Binding of water to minerals.

The fraction of water bound to the bentonite is given by

$$F_b = F_w(S_w)Th(T) \quad (3.4.2)$$

where F_b is the fraction of water in compartment bound to bentonite (-), $F_w(S_w)$ is an empirical function giving the fraction of water bound to bentonite as a function of temperature (range 0-1) (-), and $Th(T)$ is an empirical parameter scaling the fraction of water bound by temperature (range 0-1) (-).

This relationship is intended to provide a simple representation of a more complex series of processes. The calculated fraction of bound water is used in the hydraulic model to scale fluid transfer fluxes and hence ensure physically appropriate amounts of water are available for transport in the system.

3.5. CU (COMPASS).

The improvements proposed by Cardiff University focus on:

- Inclusion of osmotic potential phenomena.
- Explicit form of thermal diffusion term in multi-component chemical transport equation.
- Inclusion of high temperature phenomena.
- Inclusion of biological impacts.
- Introducing HPC techniques to THMC analysis.

The mathematical formulation of those improvements is described below:

3.5.1. Inclusion of osmotic potential phenomena

This section deals with the development of an explicit form of osmotic potential relationships for inclusion into the existing thermo-hydraulic formulation (temperature, moisture, dry air and multi-component chemical transport equations).

- **Liquid flow**

Currently, COMPASS adopts the following approach to compute the liquid velocity:

$$\mathbf{v}_l = -k_l \left\{ \nabla \left(\frac{u_l}{\gamma_l} \right) + \nabla z \right\} + \sum_{i=1}^{nc} K_l^{c_d^i} \nabla c_d^i \quad (3.5.1)$$



The objective of this section is to re-derive equation (3.5.1) by taking into consideration the definition of osmotic potential, so as to provide an alternative to the $K_l^{c_d}$ term in equation (3.5.1).

Following Darcy's law, the velocity of liquid flow can be defined as:

$$\mathbf{v}_l = -k_l i_h \quad (3.5.2)$$

where the hydraulic gradient, i_h , is expressed as:

$$i_h = \nabla \psi_m + \nabla \psi_g + \nabla \psi_o \quad (3.5.3)$$

where $\nabla \psi_m$ is the gradient due to matric potential, $\nabla \psi_g$ is the gradient due to elevation and $\nabla \psi_o$ is the gradient due to osmotic potential. The first two terms is as defined in equation (3.5.1). Therefore, the key steps in the derivation of only $\nabla \psi_o$ term will be described below. The methodology has been adopted from Wu and Chieng (1995):

$$\nabla \psi_o = \sum_{i=1}^{nc} \frac{\partial \psi_o}{\partial c_d^i} \nabla c_d^i + \frac{\partial \psi_o}{\partial T} \nabla T \quad (3.5.4)$$

ψ_o can be defined as (Zelinchenko and Sokolenko, 1986):

$$\psi_o = \frac{-1000RT\omega \sum_{i=1}^{nc} A_i}{\rho_l g} \quad (3.5.5)$$

where ω is the osmotic efficiency, A_i is the activity of the i^{th} component, nc is the total number of chemical components in the pore water, ρ_l is the density of liquid moisture, g is the gravitational constant, R is the gas constant and T is the temperature.

The activity, A_i , can be defined as:

$$A_i = \gamma_i c_d^i \quad (3.5.6)$$

where γ_i is the activity coefficient of the i^{th} chemical component.

Combining equations (3.5.4) and (3.5.5) into (3.5.3) yields:

$$i_h = \frac{\nabla u_l}{\gamma_l} + \nabla z + \sum_{i=1}^{nc} \frac{-1000RT\gamma_i\omega_o}{\rho_l g} \nabla c_d^i + \frac{-1000R\omega_o}{\rho_l g} \sum_{i=1}^{nc} \gamma_i c_d^i \nabla T \quad (3.5.7)$$

Substituting equation (3.5.7) into (3.5.2) yields:

$$\mathbf{v}_l = -k_l \left[\frac{\nabla u_l}{v_l} + \nabla z + \sum_{i=1}^{nc} \frac{-1000RT\gamma_i\omega_o}{\rho_l g} \nabla c_d^i + \frac{-1000R\omega_o}{\rho_l g} \sum_{i=1}^{nc} \gamma_i c_d^i \nabla T \right] \quad (3.5.8)$$

- **Vapour flow**

In the existing model, the velocity of vapour is defined by both Philip and de Vries (1957) and Ewen and Thomas (1989) approach. In the first instance, the inclusion of osmotic effect will be demonstrated for the Philip and de Vries case:

$$\mathbf{v}_v = -\frac{D_{atms} v_v \tau_v \theta_a}{\rho_l} \nabla \rho_v \quad (3.5.9)$$

where ρ_l is the density of liquid moisture, D_{atms} is the molecular diffusivity of vapour through air, v_v is a mass flow factor, τ_v is the tortuosity factor, θ_a is the volumetric air content and $\nabla \rho_v$ is the vapour density gradient.

The term ρ_v was originally defined as:

$$\rho_v = \rho_o h \quad (3.5.10)$$

where ρ_o is the density of saturated water vapour and h is the relative humidity in the pore space. Note that there was no distinction made between relative humidity due to matric or osmotic potential terms in the above equation.

The modification of equation (3.5.10) due to osmotic potential can be expressed as:

$$h = h_m h_o \quad (3.5.11)$$

where h_m is the relative humidity due to matric potential and h_o is the relative humidity due to osmotic potential.

Substituting equation (3.5.11) into equation (3.5.10) and differentiating yields:

$$\nabla \rho_v = \rho_o [h_o \nabla h_m + h_m \nabla h_o] \quad (3.5.12)$$

The derivation will now focus upon the second term

$$\begin{aligned} \nabla \rho_v = \rho_o h_o \left[\frac{\partial h_m}{\partial s} \nabla s + \frac{\partial h_m}{\partial T} \nabla T \right] + \rho_o h_m \sum_i^{nc} \frac{\partial h_o}{\partial c_d^i} \nabla c_d^i \\ + \rho_o h_m \frac{\partial h_o}{\partial T} \nabla T + h_m h_o \frac{\partial \rho_o}{\partial T} \nabla T \end{aligned} \quad (3.5.13)$$

where s is the suction.

The term h_o can be defined as:

$$h_o = \exp\left(\frac{M \psi_o g}{RT}\right) \quad (3.5.14)$$

where $M = 0.018015$ kg/mol, g is the gravitational constant, R is the gas constant and T is the temperature.

Substituting equation (3.5.13) into (3.5.9) yields:

$$\mathbf{v}_v = -\frac{D_{atms} v_v \tau_v \theta_a}{\rho_l} \nabla \cdot \left\{ \begin{aligned} &\rho_o h_o \left[\frac{\partial h_m}{\partial s} \nabla s + \frac{\partial h_m}{\partial T} \nabla T \right] + \rho_o h_m \sum_i^{nc} \frac{\partial h_o}{\partial c_d^i} \nabla c_d^i \\ &+ \rho_o h_m \frac{\partial h_o}{\partial T} \nabla T + h_m h_o \frac{\partial \rho_o}{\partial T} \nabla T \end{aligned} \right\} \quad (3.5.15)$$

• Implications on the governing equations

The basic form of moisture (liquid + vapour), dry air, heat and multi-component chemical transport equations are presented below (Thomas et al., 1998; Cleall et al. 2007a; Cleall et al. 2007b):

Liquid moisture:

$$\rho_l \frac{\partial n S_l}{\partial t} + \frac{\partial \rho_v n S_a}{\partial t} = -\rho_l \nabla \cdot \mathbf{v}_l - \rho_l \nabla \cdot \mathbf{v}_v - \nabla \cdot (\rho_v \mathbf{v}_a) \quad (3.5.16)$$

Dry air:

$$\frac{\partial [\theta_a + H_s \theta_l] \rho_{da}}{\partial t} = -\nabla \cdot [\rho_{da} (\mathbf{v}_a + H_s \mathbf{v}_l)] \quad (3.5.17)$$

Heat:

$$\frac{\partial (H_c (T - T_r) + Ln S_a \rho_v)}{\partial t} = -\nabla \cdot \left[-\lambda_T \nabla T + (\mathbf{v}_v \rho_v + \mathbf{v}_a \rho_a) L + (C_{pl} \mathbf{v}_l \rho_l + C_{pv} \mathbf{v}_v \rho_l + C_{pv} \mathbf{v}_a \rho_v + C_{pda} \mathbf{v}_a \rho_{da}) (T - T_r) \right] \quad (3.5.18)$$

Multi-component chemical:

$$\frac{\partial (\theta_l c_d^i)}{\partial t} + \frac{\partial (\theta_l s_i)}{\partial t} = -\nabla \cdot (c_d^i \mathbf{v}_l - \theta_l D_i \nabla c_d^i + \theta_l D_i S_i c_d^i \nabla T) \quad (3.5.19)$$

The \mathbf{v}_l , ρ_v and \mathbf{v}_v terms in the above equations are substituted by equations (3.5.8), (3.5.15) and (3.5.10) respectively.

3.5.2. Explicit form of thermal diffusion term in multi-component chemical transport equation

The governing equation for the multi-component chemical transport in the COMPASS model is expressed as:

$$\frac{\partial (\theta_l c_d^i)}{\partial t} + \frac{\partial (\theta_l s_i)}{\partial t} = -\nabla \cdot (c_d^i \mathbf{v}_l - \theta_l D_i \nabla c_d^i + \theta_l D_i S_i c_d^i \nabla T) \quad (3.5.20)$$

where θ_l is volumetric water content, c_d^i is the total dissolved concentration, s_i is the sink/source term evaluated using MINTEQA2 (Allison et al. 1991), \mathbf{v}_l is the Darcy's velocity vector, D_i is the apparent diffusion coefficient, S_i is the Soret coefficient, and T is the temperature. The subscript "i" represents the i^{th} chemical component. The second term in equation (3.5.20) is referred to as the thermal diffusion term. In this report, discussions on mechanical dispersion are ignored considering that the transport through bentonite is diffusion dominated.

The objective of this work is to derive an alternative expression for the thermal diffusion term. The work that follows has been mainly adopted from the theory of electrochemistry (Bockris and Reddy, 2002; Sansom et al., 2007).

Equation (3.5.20) is essentially the Fick's second law of diffusion with additional terms to account for advective velocity and sink/source. Re-deriving the second law via the use of chemical potential relationship will enable determination of an explicit form of relationship for the thermal diffusion term.

The diffusion ionic flux can be defined as:

$$j_i = \frac{-D_i^o}{RT} c_d^i \nabla (\mu_i) \quad (3.5.21)$$



where D_i^o is the diffusion coefficient in free solution, R is the gas constant, T is the temperature, c_d^i is the total dissolved concentration, μ_i is the electrochemical potential and \mathbf{v}_l is the velocity of liquid. The first term represents diffusion and the second advection.

The electrochemical potential term, μ_i , can be defined as:

$$\mu_i = \mu_i^o + RT \ln(\gamma_i c_d^i) + z_i F \psi \quad (3.5.22)$$

where μ_i is the electrochemical potential, μ_i^o is the reference value of μ_i , γ_i is the activity coefficient, z_i is the valence number, F is the Faraday's constant and ψ is the electrodiffusion potential.

The gradient of μ_i can be defined as:

$$\nabla \mu_i = \frac{\partial \mu_i}{\partial c_d^i} \nabla c_d^i + \frac{\partial \mu_i}{\partial T} \nabla T \quad (3.5.23)$$

Ignoring the electrodiffusion term, equation (3.5.22) can be recast as:

$$\mu_i = \mu_i^o + RT \ln(c_d^i) + RT \ln(\gamma_i) \quad (3.5.24)$$

Differentiating equation (3.5.24) w.r.t. c_d^i yields:

$$\frac{\partial \mu_i}{\partial c_d^i} = \frac{RT}{c_d^i} + RT \frac{\partial \ln \gamma_i}{\partial c_d^i} = \frac{RT}{c_d^i} \left[1 + \frac{\partial \ln \gamma_i}{\partial \ln c_d^i} \right] \quad (3.5.25)$$

Differentiating equation (3.5.24) w.r.t. T yields:

$$\frac{\partial \mu_i}{\partial T} = R \ln(\gamma_i c_d^i) \quad (3.5.26)$$

Combining (3.5.25) and (3.5.26) into (3.5.23) yields:

$$\nabla \mu_i = \frac{RT}{c_d^i} \left[1 + \frac{\partial \ln \gamma_i}{\partial \ln c_d^i} \right] \nabla c_d^i + R \ln(\gamma_i c_d^i) \nabla T \quad (3.5.27)$$

Substituting (3.5.27) into (3.5.21) gives:

$$j_i = \frac{-D_i^o}{RT} c_d^i \left\{ \frac{RT}{c_d^i} \left[1 + \frac{\partial \ln \gamma_i}{\partial \ln c_d^i} \right] \nabla c_d^i + R \ln(\gamma_i c_d^i) \nabla T \right\} \quad (3.5.28)$$

Simplifying further:

$$j_i = -D_i^o \left(1 + \frac{\partial \ln \gamma_i}{\partial \ln c_d^i} \right) \nabla c_d^i - \frac{D_i^o c_d^i}{T} \ln(\gamma_i c_d^i) \nabla T \quad (3.5.29)$$

In macroscopic terms, equation (3.5.29) can be recast as:

$$j_i = -\theta D_i \left(1 + \frac{\partial \ln \gamma_i}{\partial \ln c_d^i} \right) \nabla c_d^i - \frac{\theta D_i c_d^i}{T} \ln(\gamma_i c_d^i) \nabla T \quad (3.5.30)$$

Including the advective velocity, equation (3.5.30) becomes:

$$j_i = -\theta D_i \left(1 + \frac{\partial \ln \gamma_i}{\partial \ln c_d^i} \right) \nabla c_d^i - \frac{\theta D_i c_d^i}{T} \ln(\gamma_i c_d^i) \nabla T + c_d^i \mathbf{v}_l \quad (3.5.31)$$

Comparison of the RHS of the main governing equation with (3.5.31) provides the explicit form of Soret coefficient term, i.e.

$$S_i = \frac{c_d^i}{T} \ln(\gamma_i c_d^i) \quad (3.5.32)$$

The other modification that can be noted is the $\frac{\partial \ln \gamma_i}{\partial \ln c_d^i}$ term, which is attributed to the ionic strength effect. Usually, this term is ignored when dilute concentration is assumed to exist in the pore water. However, in this formulation, this term is active as higher ionic strengths are allowed.

3.5.3. Inclusion of high temperature phenomena.

Current capability of the THMC formulation in the COMPASS model is limited to temperatures less than 100°C, therefore suitable modifications undertaken to address this limitation has been presented in this section. In the following paragraphs only the modifications to the THM governing equations are dealt.

Pore air velocity:

At higher temperatures vapour flow occurs due to a high bulk air pressure gradient (Luikov, 1954), which may have significant influence on the vapour flux. Therefore, bulk air velocity can be expressed via Darcy's law (Luikov, 1954).

$$\mathbf{v}_g = -K_g \nabla P_g \quad (3.5.33)$$

where \mathbf{v}_g is velocity of pore air, K_g is air conductivity and P_g is pore air pressure. The total air pressure is also a function of temperature and follows the approach of Geraminegad and Saxena (1986). Thus equation (3.5.33) can be expressed as:

$$\mathbf{v}_g = -K_g \left[\frac{\partial P_g}{\partial T} \nabla T + \nabla P_g \right] \quad (3.5.34)$$

Air conservation:

To consider the high temperature effect on the air conservation equations several modifications are made such as: a sink/source term is introduced in the air transfer equation followed by Luikov (1954), also pressure-temperature relationship in both storage and flux terms are used based on Geraminegad and Saxena (1986). Hence the modified air transfer equation can be represented as follows:

$$\frac{\partial}{\partial t} [\rho_{da} \theta_g + \rho_{da} H \theta_l] = -\nabla \cdot [\rho_{da} \mathbf{v}_g + \rho_{da} H \mathbf{v}_l] + \nabla \cdot \mathbf{J}_v \quad (3.5.35)$$

where ρ_{da} is the density of dry air, H is Henry's volumetric coefficient of solubility and \mathbf{J}_v is the sink/source term.

Energy conservation:

$$\frac{\partial(\Omega)}{\partial t} = -\nabla \cdot \mathbf{Q} \quad (3.5.36)$$

where Ω is the heat content and \mathbf{Q} is the heat flux.

Heat content can be defined as;

$$\Omega = H_c(T - T_r) + nLS_g\rho_v \quad (\text{J/m}^3) \quad (3.5.37)$$

where L is the latent heat of vaporisation.

However, the heat capacity of unsaturated soil, H_c , at reference temperature, T_r , may be defined as;

$$H_c = (1-n)C_{ps}\rho_s + n(C_{pl}S_l\rho_l + C_{pv}S_g\rho_v + C_{pda}S_g\rho_{da}) \quad (\text{JK/m}^3) \quad (3.5.38)$$

where C_{ps} , C_{pl} , C_{pv} , and C_{pda} are the specific heat capacities of solid particles, liquid, vapour, and dry air respectively and ρ_s is the density of solid particles. C_{pl} , C_{pv} , and C_{pda} are functions of temperature and represented by polynomial equations as follows according to Pakowski *et al.* (1991).

$$C_{pl} = \sum_{i=0}^n a_i T(K)^i \quad (3.5.39)$$

$$C_{pv} = \sum_{i=0}^n a_i T(K)^i \quad (3.5.40)$$

$$C_{pda} = \sum_{i=0}^n a_i T(^{\circ}\text{C})^i \quad (3.5.41)$$

where a is coefficient, values of which are given in a tabular form, $T(K)$ temperature in Kelvin and $T(^{\circ}\text{C})$ temperature in degree centigrade.

Deformation behaviour:

The existing deformation model in COMPASS (Thomas and He, 1995) considers temperature effect on the stress-strain relationship as follows;

$$d\varepsilon = d\varepsilon_{\sigma} + d\varepsilon_T + d\varepsilon_s \quad (3.5.42)$$

where ε is the strain and the subscripts σ , T , s refer to net stress, temperature and suction contributions.

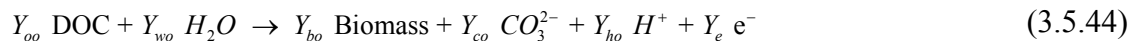
Additionally, a relation between stress and suction due to increase in cohesion and changes of temperature is adopted from Gens et al., (1995) as follows;

$$p_s = kse^{-\rho\Delta T} \quad (3.5.43)$$

where k and ρ are model parameters, p_s parameter controlling suction effects on cohesion, s suction and ΔT increase of temperature. However, the applicability of the above term for higher temperatures, i.e. beyond 100 °C needs to be examined.

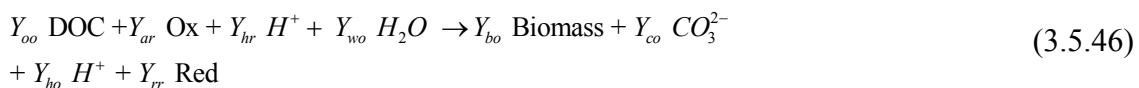
3.5.4. Inclusion of biological impacts

The approach adopted in this research follows that proposed by Brun and Engesgaard (2002). In terms of the conceptualisation of microbial species, a macroscopic approach is adopted which does not consider any structural arrangement of the microbial population. In other words, they are treated as a bulk averaged quantity. In terms of the type of biodegradation models, a multiplicative Monod kinetic model is applied keeping in mind the range of substrate concentrations that may occur in real systems. In terms of the coupling of biodegradation reactions with inorganic chemistry, a two-step partial equilibrium approach has been adopted. The two-step process writes a degradation reaction as two-half cell reactions. An example is as shown below (Brun et al. 1994):



where Y_{ij} denotes the stoichiometric coefficient of species i in reaction j . The first reaction is treated as kinetically controlled and hence a multiplicative Monod kinetic model is applied, whilst the second reaction is considered to be an equilibrium reaction and hence handled via an equilibrium geochemical model. In this instance, MINTQA2 (Allison et al. 1991) is used.

The overall biodegradation reaction will then be:



The assumptions are that microbes are immobile and changes to porous medium porosity or permeability due to microbial population are neglected. Adopting therefore Brun and Engesgaard's (2002) approach, the biodegradation rate of an organic compound is described via the following multiplicative Monod equation:

$$q_i = R_i I_i \left(\frac{[\text{DOC}]}{K_{\text{DOC}} + [\text{DOC}]} \right) \left(\frac{[ea_i]}{K_{ea} + [ea_i]} \right) \quad (3.5.47)$$

$$q_{b,i} = \frac{d[b_i]}{dt} = [b_i](Y_{bo}q_i - d_i) \quad (3.5.48)$$

where q_i is the specific biomass formation rate, $q_{b,i}$ is the rate of biomass growth, R_i is the maximum process rate of biomass, d is the decay rate of biomass, $[ea_i]$ is the concentration of electron acceptors, $[DOC]$ is the concentration of dissolved organic carbon, $[b_i]$ is the biomass concentrations, K_{ea} is the half saturation constants for the current electron acceptor, K_{DOC} is the half saturation constants for dissolved organic carbon and ab is the biomass stoichiometric coefficient. The inhibition function I_i is evaluated via:

$$I_i = 1, \text{ if } [ea_i] \frac{[k_i]}{[k_i]} \geq [k_i], \text{ else } I_i = 0 \quad (3.5.49)$$

where $[k_i]$ represents the inhibition constant for the inhibiting electron acceptors i . The inhibiting function accounts for inhibition of the weaker-oxidising electron acceptors by the stronger oxidising electron acceptor present in solution. When biomass is produced the associated change in the DOC concentration is:

$$q_{DOC} = \frac{d[DOC]}{dt} = -\sum_{i=1}^{M_b} Y_{oo}q_i \quad (3.5.50)$$

where q_{DOC} is the rate of consumption of DOC. Similarly the associated change in other reactants and products of any biodegradation reaction can be evaluated based on their stoichiometries and q_i .

Biodegradation reactions can produce or consume alkalinity, thereby initiating changes in solution chemistry. Therefore, the influence of biodegradation reactions on the inorganic chemistry will be considered. This is achieved by linking the outputs from the biodegradation model with the geochemical model, MINTEQA2 (Islam and Singhal, 2002).

The redox potential (pE) is estimated at each location of the domain based on the concentrations of the dominant terminal electron acceptor and its corresponding reduced species from the transport and kinetic biodegradation model (Smith and Jaffe 1998; Islam and Singhal, 2002). Together with other computed species concentrations the estimated pE can then be used in the chemical equilibrium model to calculate the equilibrium state towards which the system should be driven.

Equation (3.5.19) presented the multi-component reactive chemical transport equation which represents transport of all aqueous geochemical components, including the relevant electron acceptors and dissolved organic matter. The sink/source term essentially addresses change in chemical concentrations due to adsorption and mineral precipitation/dissolution. With respect to precipitation/dissolution reactions, EAs are relevant and their transport is governed by their primary variables, depending upon the solubility constants and the geochemical environment. However, the changes in concentrations due to biodegradation reactions are solved independently of equation (3.5.19) and linked back to the geochemical model.



3.5.5. Introducing HPC techniques to THMC analysis

This section presents some of the recent advances in high performance computing (HPC) techniques at the Geoenvironmental Research Centre being adapted to the THMC framework. To reduce the time of calculation a high performance computation is proposed defined as the implementation of a parallel processing algorithm. In the following schema a comparison is given between a serial and a parallel calculation.

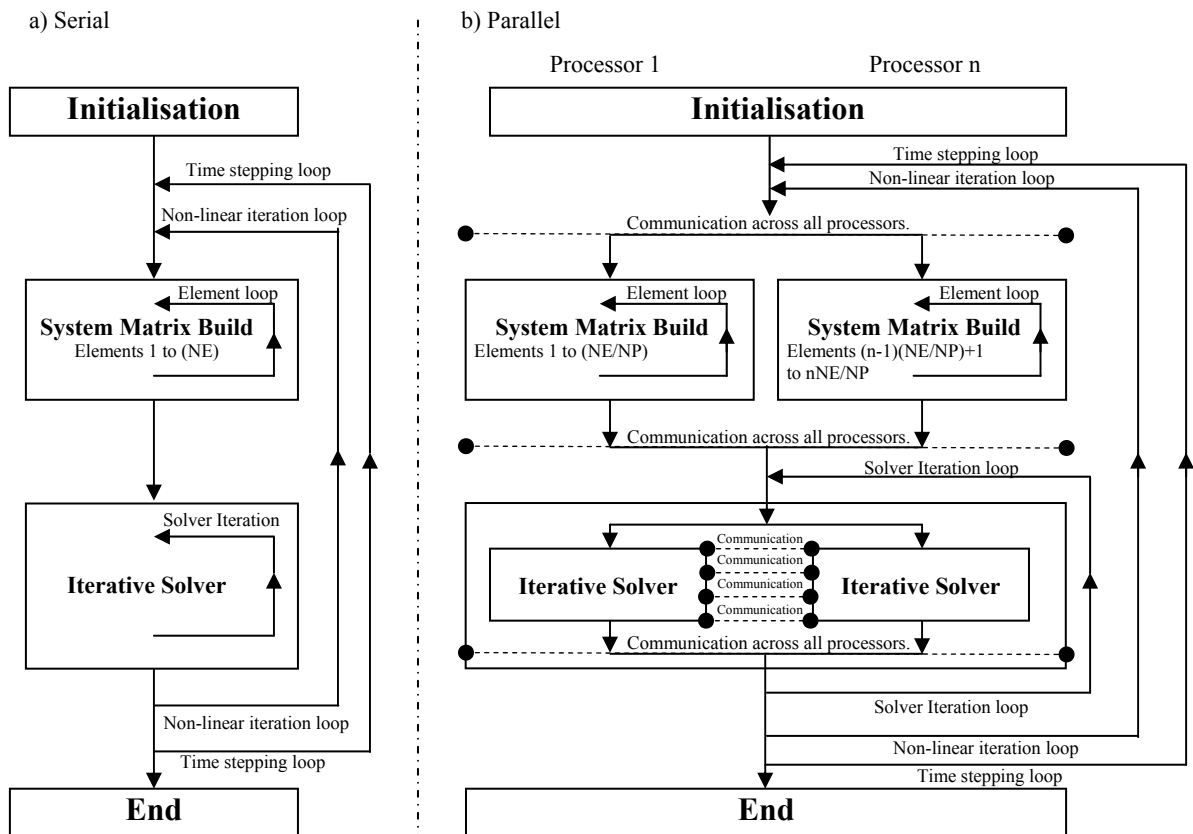


Figure 1 – Schematic of the main areas of computation with NE elements on NP processors.

3.6. IRSN (CAST3M).

As far as THM calculations are concerned, one major interest of Cast3m is to make available thermal and hydromechanical analysis modules in the same computer program, thus enabling coupled calculations when necessary. For example, in the case of saturated media, mixed finite elements are used, in which the displacements are interpolated using quadratic polynomials, whereas the fluid pressure is interpolated using linear polynomials. The Galerkin method is used to solve in a weak form the mass balance and momentum equations. For the time integration, a classical θ method is used.

In order to solve the THM problem, an incremental approach is implemented in a CAST3M procedure. For each time step, this procedure calls another procedure, which solves the non linear equations in an iterative way. The iterations are performed until the various residuals are lower than some user prescribed tolerances. In the case of a THM problem, the thermal analysis is done first. It can use a mesh different from the mechanical one. The temperature fields are then projected on the mechanical mesh. Then, the HM problem step is solved. Iterations between T and HM problems are possible at each time step.

For the solution of both T and HM non linear algebraic systems, a Newton-Raphson method is used, with different possible variants such as tangent stiffness, initial stiffness, convergence acceleration techniques, etc. Moreover, the linear algebraic system can be solved either directly (Crout method) or iteratively (conjugate gradient method).

In the framework of the THERESA project, the first calculations have shown at least two limitations of CAST3M: the material model used for the bentonite is a linear elastic one and the thermal vapor diffusivity used is too large in case of low saturations. Therefore, two developments are considered necessary:

- a. Implementation of a non linear elastic material model for bentonite.
- b. Introduction of a saturation dependent reducing factor on the thermal vapour diffusivity.



4. Summary of codes and formulations. Concluding remarks

Tables 2, 3 and 4 summarise the main features of the codes included in WP4. It should be pointed out that those Tables correspond to the state of the codes described in the initial reports and not to the final state at the end of the project.

Table 2 lists the balance equation considered by the various formulations as well as the level of integration adopted. It can be observed that all codes include the balance equations if water and energy (required for non-isothermal cases) and equilibrium. Not all codes, however, consider the air mass balance equation. This absence is not important in most cases as the air pressure can be considered in equilibrium with atmospheric pressure. It may be required, however in confined problems or when high temperatures are reached. Coupled formulations are used throughout except in the case of CAST3M where the thermal problem is treated uncoupled from the coupled HM component. In the fully coupled formulations, both monolithic and staggered approaches are adopted.

The main constitutive equations are collected in Table 3 where the stress variables used are also listed. Various mechanical models are employed although they generally include a component to deal with the strong swelling properties of the bentonite. Most codes adopt a generalised Darcy's law for liquid flow but there is more variety concerning the description of vapour diffusion.

Finally Table 4 indicates which relevant processes are considered in the various formulations. It is worth noting that all formulations incorporate vapour flow, an essential ingredient in non-isothermal problems especially when dealing with unsaturated conditions. There is more variety in the consideration of heat advection, latent heat and gas flow. It is also interesting to note that four out of six codes include the possibility to deal with geochemical processes.

It can thus be concluded that the formulations adopted place the codes in a good position for a successful modelling of the coupled THM processes in the buffer. Less attention is given to the explicit modelling of the interfaces. THMC analyses are in principle feasible for four of the codes. In spite of the quite powerful initial formulations of all the codes, an impressive array of proposed improvements has been put forward by the various teams.



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Table 2. Codes and formulations.

Group	Code	Balance equation				Type of formulation
		Water	Air	Energy	Equilib.	
CIMNE	Code_Bright	Y	Y	Y	Y	Monolithic coupled
Posiva/Marintel	FreeFEM++	Y	N	Y	Y	Staggered coupled
KTH	ROLG	Y	Y	Y	Y	Monolithic coupled
Quintessa	QPAC-EBS	Y	Y	Y	Y	Monolithic coupled
Cardiff University	COMPASS	Y	Y	Y	Y	Monolithic coupled
IRSN	CAST3M	Y	N	Y	Y	Staggered coupled

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Table 3: Constitutive equations.

Group	Code	Mechanical	Stress Variables	Liquid flow	Vapour diffusion
CIMNE	Code_Bright	Barcelona Basic Model (BBM)	Net stress (unsat) Effective Stress (sat)	Generalized Darcy	Fick (+tortuosity)
Posiva/Marintel	FreeFEM++	Poroelastic model	Total (net) stresses	Moisture diffusion	Vapour flow function (related to hyd. cond.)
KTH	ROLG	Elasticity +swelling pressure	Biot coefficient	Generalized Darcy	Driven by thermal gradient
Quintessa	QPAC-EBS	Viscoelasticity+swelling pressure	Effective Stress	Generalized Darcy	Fick (+interface area)
Cardiff University	COMPASS	Elastoplastic model	Net stress (unsat)	Generalized Darcy	Based on Philip and de Vries (1957)
IRSN	CAST3M	Elastic+swelling pressure	Biot coefficient (unsat)	Generalized Darcy	Fick(+tortuosity)

[THERESA]

Table 4: Phenomena included in the formulation.

Group	Code	Heat Transport				Liquid flow		Air flow	Mechanical Behaviour		Geochemical process
		Cond.	Adv.(l)	Adv (v)	Latent heat	Liquid	Vapour	Gas	Therm. Expan.	Suction effect	
CIMNE	Code_Bright	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
Posiva/Marintel	FreeFEM++	Y	N	N	N	Y	Y	N	N	Y	Y
KTH	ROLG	Y	Y	N	N	Y	Y	Y	Y	Y	N
Quintessa	QPAC-EBS	Y	Y	Y	N*	Y	Y	Y	N*	Y	Y
Cardiff University	COMPASS	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
IRSN	CAST3M	Y	N	N	N	Y	Y	N	Y	Y	N

(*) Those processes can be modelled but they were turned off as they were not considered important in the tests cases

[THERESA]

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