Numerical Implementation of a Multivariable Thermomechanical Model for Unsaturated Bentonite

Veli-Matti Pulkkanen*[1] and Markus Olin[1]

[1] VTT Technical Research Center of Finland

*Otakaari 3 K, Espoo, P.O. Box 1000, FI-02044 VTT, Finland, veli-matti.pulkkanen@vtt.fi

Abstract: A compacted bentonite clay buffer is planned to be used as a part of the engineered barrier system in the KBS-3 concept for the disposal of spent nuclear fuel. Simulations together with experimental studies are needed to ensure that bentonite fulfills its safety functions in the concept. In this paper, one type of bentonite model, namely a thermomechanical model developed by Petri Jussila, is presented in brief and its numerical implementation with COMSOL Multiphysics 4.0a is discussed. The model describes bentonite as a mixture of four components: solid skeleton, liquid water, water vapour, and air. The system is defined by basic balance laws along with the somewhat complex constitutive equations that are based on a thermomechanical approach. Previously, the model has been implemented with software called Elmer by CSC – IT Center for Science and with an in-house code Numerrin by Numerola Oy that has made some extensions to the model.

Keywords: bentonite, saturation, thermomechanics

1. Introduction

A compacted bentonite clay buffer is planned to be used as a part of the engineered barrier system in the KBS-3 concept for the disposal of spent nuclear fuel (Figure 1). After installation, the compacted bentonite buffer should swell to isolate the canister from flowing groundwater. On the other hand, the buffer should still stay loose enough to protect the canister from mechanical disturbances. In order to meet these two needs, both experimental and modeling studies have to be carried out. In this paper, a thermomechanical approach of modeling the saturation of the buffer is considered. The somewhat complex model that is presented here is developed by Petri Jussila and we advise the interested reader to see [1], [2], and [3] for details.

In the model, water can enter the pore space of a solid skeleton of the bentonite as liquid or vapor. Also the evaporation of the liquid water is considered in the model since in reality the water can evaporate near the canister that is heated by the decaying spent nuclear fuel. Water vapor form the gas phase of the model together with air. Moreover, the solid skeleton can deform and develop stress due to the incoming water. Thereby, the model includes deformation and transport of the four constituents according to balances of mass, linear momentum, and energy that are completed by constitutive laws.
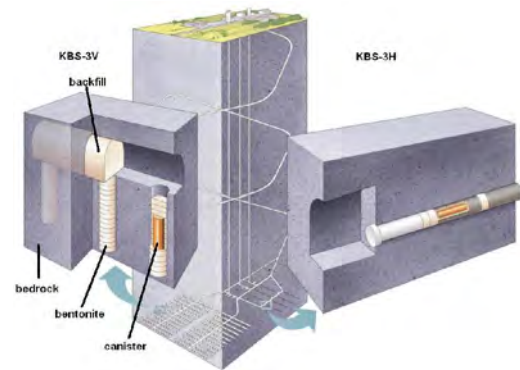

Figure 1. A schematic figure of the KBS-3 disposal concept. [4]

2. Theory

In this section, we describe the steps to derive the final equations of the model. The steps are: choosing the variables of the system, writing the balance laws, describing a procedure to derive thermodynamically consistent constitutive equations from the free energies and the dissipation function, choosing the free energies and the dissipation function, and, finally, substituting the material laws into the simplified final equations.

2.1 Constituents, the state and the dissipative variables

In the model, the constituents of bentonite are solid skeleton (s), liquid water (l), water vapor (v) and air (a). Their molar volume fractions are ξ_s, ξ_l, ξ_v, and ξ_a, respectively. The fractions have to be positive and add up to one, that is:

$$\xi_k \geq 0 \text{ for k=s,l,v,a and}$$

$$\xi_s + \xi_l + \xi_v + \xi_a = 1.$$

The other state variables are the intrinsic (or bulk) densities $\tilde{\rho}_k$, the strain ϵ, and the temperature T. The dissipative variables (the rate of deformation $\mathbf{D}$, velocities $\mathbf{U}_k$, heat flux $\mathbf{q}$, and evaporation rate $-\theta_l$), of the system describe the dissipative behavior of the system.

2.2 Balance laws

Balance laws for the mass of solid, liquid water, water vapor, air, linear momentum, and energy are simply:

$$\frac{\partial \rho_s}{\partial t} + \nabla \cdot (\rho_s \mathbf{U}_s) = 0.$$

$$\frac{\partial \rho_l}{\partial t} + \nabla \cdot (\rho_l \mathbf{U}_l) = \theta_l$$

$$\frac{\partial \rho_v}{\partial t} + \nabla \cdot (\rho_v \mathbf{U}_v) = -\theta_l$$

$$\frac{\partial \rho_a}{\partial t} + \nabla \cdot (\rho_l \mathbf{U}_a) = 0$$

$$-\nabla \cdot \sigma - \rho_s \mathbf{g} = 0$$

$$(\rho c)_{\text{eff}} \frac{\partial T}{\partial t} - (e_v - e_l)\theta_l - \nabla \cdot (\lambda \nabla T) = 0$$

where ρ_k are the apparent densities of the constituents, σ the Cauchy stress tensor, $\mathbf{g}$ the gravitational acceleration, $(\rho c)_{\text{eff}}$ the effective specific heat, $e_v - e_l$ the internal energy difference of the liquid water and vapor, and λ the total heat conductivity. The apparent densities relate to intrinsic (or bulk) densities by $\rho_k = \xi_k \tilde{\rho}_k$. For solid and liquid the bulk densities are constant while for gases they are

$$\tilde{\rho}_k = \frac{\hat{B} M_k}{RT} \text{ where } \hat{B} \text{ is the gaseous pressure.}$$

2.3 General constitutive relations

In this section, we describe a procedure that can be used to derive constitutive equations which do not violate the second law of thermodynamics. As a result of the procedure, the constitutive laws can be obtained by defining only the constituent free energies ψ_k and the dissipation function ϕ. The Clausius-Duhem inequality for mixtures is

$$\sum_k T\gamma_k = \Sigma_k \left[-\sigma_k : \mathbf{D}_k \right.$$
$$- \rho_k \left(\frac{d^k \psi_k}{dt} + s_k \frac{d^k T}{dt} \right)$$
$$- \left(\psi_k - \frac{1}{2} \mathbf{U}_k \cdot \mathbf{U}_k \right) \theta_k$$
$$\left. - \frac{\nabla T}{T} \cdot \mathbf{q}_k - \right] \geq 0$$

where γ_k is the rate of entropy production, ψ_k is the constituent k free energy and s_k the constituent specific entropy. We can define the dissipation function ϕ with this inequality by

$$\phi_{\text{C-D}} = \sum_k T\gamma_k.$$

On the other hand, the dissipation function has to obey the principle of maximal rate of entropy production. Thereby, if we have j generalized, mutually independent irreversible forces $\mathbf{X}_{k,j}$ and fluxes $\mathbf{J}_{k,j}$, the dissipation function has to be the solution to the maximum problem

$$\max \sum_{j,k} \mathbf{X}_{k,j} : \mathbf{J}_{k,j} \text{ subject to}$$

$$\phi_{\max} - \sum_{j,k} \mathbf{X}_{k,j} : \mathbf{J}_{k,j} = 0$$

.

The solution of the problem implies that the dissipation function can be expanded as

$$\phi_{\max} = \frac{v'}{1+v'} \sum_{j,k} \frac{\partial \phi}{\partial \mathbf{J}_{k,j}} : \mathbf{J}_{k,j}$$

where v' is the Lagrangian multiplier of the maximum problem. If the dissipation function is chosen to be quadratic, the coefficient $v = \dfrac{v'}{1-v'}$ becomes $\dfrac{1}{2}$. Now, using the already chosen dissipative variables and marking the dissipation defined by Clausius-Duhem inequality and the maximum principle equal, that is

$$\phi_{\text{C-D}} = \phi_{\max} \,,$$

we have the general constitutive relations that connect the state and dissipative variables to the free energies and the dissipation function. The relations are

$$\sigma_k^D = \rho_k \frac{\partial \psi_k}{\partial \epsilon_k^D} + v \frac{\partial \phi}{\partial \mathbf{D}_k^D} \,,$$

$$p_k = -\rho_k \frac{\partial \psi_k}{\partial (\text{tr}\epsilon_k)} - v \frac{\partial \phi}{\partial (\text{tr}\mathbf{D}_k)} + p_k^{\xi} \,,$$

$$s_k = -\frac{\partial \psi_k}{\partial T} \,,$$

$$p_k^{\xi} = \xi_k \Sigma_j \rho_j \frac{\partial \psi_j}{\partial \xi_k}$$

$$-\frac{\nabla T}{T} = v \frac{\partial \phi}{\partial \mathbf{q}_k}$$

$$-\sum_j \rho_k \frac{\partial \psi_k}{\partial \xi_j} \nabla \xi_j + \sum_j \rho_j \frac{\partial \psi_j}{\partial \xi_k} \nabla \xi_k = v \frac{\partial \phi}{\partial \mathbf{V}_k}$$

$$\left(\psi_i - \frac{1}{2} \mathbf{U}_v \cdot \mathbf{U}_v \right) - \left(\psi_l - \frac{1}{2} \mathbf{U}_l \cdot \mathbf{U}_l \right) = 2v \frac{\partial \phi}{\partial \theta}$$

where superscript ^{D} means deviatoric part, ρ_k^{ξ} is the interaction pressure. Now the free energies and dissipation function have to be chosen to complete the mathematical description of the system.

2.4 The constituent free energies and the dissipation function

The free energies cover the reversible individual behaviors of the constituents and their mutual interactions. Chosen interactions in the model are mixing of gaseous constituents, adsorption and swelling between the liquid and solid constituents. The specific free energies are for solid:

$$\psi_s(\epsilon, \xi_j, \tilde{\rho}_s, T) = \psi_{s,0} - s_{s,0}(T - T_0)$$

$$+ c_s^v (T - T_0) - c_s^v T \ln \frac{T}{T_0} + TJ(\tilde{\rho}_s)$$

$$+ \frac{1}{\tilde{\rho}_s} G(\xi_s, \xi_l) \epsilon^D : \epsilon^D$$

$$+ \frac{1}{2\tilde{\rho}_s} K(\xi_s, \xi_l)(\text{tr}\epsilon)^2$$

$$+ \frac{1}{\tilde{\rho}_s} f_{\Pi}(\xi_s, \xi_l) \hat{B}_0 \text{tr}\epsilon + \frac{T}{\tilde{\rho}_s} I(\xi_j) \,.$$

For liquid:

$$\psi_l(\xi_j, \tilde{\rho}_l, T) = \psi_{l,0} - s_{l,0}(T - T_0)$$

$$+ c_l^v (T - T_0) - c_l^v T \ln \frac{T}{T_0} + TJ(\tilde{\rho}_l)$$

$$+ \frac{RT}{M_v} f(\xi_s, \xi_l) + \frac{T}{\tilde{\rho}_l} I(\xi_j).$$

And for gases (k = v,a)

$$\psi_k(\xi_j, \tilde{\rho}_k, T) = \psi_{k,0} - s_{k,0}(T - T_0)$$

$$+ c_k^v (T - T_0) - c_k^v T \ln \frac{T}{T_0} + \frac{RT}{M_k} \ln \left(\frac{\tilde{\rho}_k}{\tilde{\rho}_{k,0}} \right)$$

$$+ \frac{RT}{M_k} \ln \left(\frac{\xi_k}{\xi_a + \xi_v} \Big/ \left(\frac{\xi_k}{\xi_a + \xi_v} \right)_0 \right) + \frac{T}{\tilde{\rho}_k} I(\xi_j)$$

Here c_k^v is the specific heat at constant volume, G the glide modulus, K the bulk modulus, M_k the molar mass, R the universal gas constant, f an adsorption function, f_Π a swelling function, and $\hat{B}_0$ is a reference pressure. I is the indicator function taking care of the restrictions for the volume fractions:

$$I = \begin{cases} 0 & \text{if } \sum_k \xi_k = 1 \text{ and } \xi_k \geq 0, \\ +\infty & \text{otherwise} \end{cases},$$

where $k \in \{s,l,v,a\}$. The other indicator function J restricts the changes in the constant intrinsic densities of the solid and the liquid water:

$$J = \begin{cases} 0 & \text{if } \tilde{\rho}_k = \tilde{\rho}_{k,0} \\ +\infty & \text{otherwise} \end{cases}.$$

The mixing interaction of the gaseous constituents is described in the terms including multiplier RT/M_k. The term that includes adsorption function defines the energy that is restored in the adsorption mechanism. Moreover, the term that includes the swelling function describes how the energy is stored to the solid when the solid swells. The shapes of the functions are discussed below.

The chosen dissipation function is

$$\phi(\mathbf{q}_k, \mathbf{V}_l, \mathbf{V}_v, \mathbf{V}_a) = \sum_{k=s,l,v,a} \frac{1}{\xi_k \lambda_k T} \mathbf{q}_k \cdot \mathbf{q}_k$$

$$+ \sum_{k=l,g} \frac{\mu_k}{k_k}(\beta_k \mathbf{V}_k) \cdot (\beta_k \mathbf{V}_k)$$

$$+ \tilde{\rho}_v \frac{RT}{M_v} \frac{1}{D} \frac{\beta_g}{\zeta(a-\zeta)}(\zeta \mathbf{V}_{vg}) \cdot (\zeta \mathbf{V}_{vg})$$

where λ_k is the thermal conductivity, μ_k the dynamic viscosity, k_k the permeability, $\beta_g = \xi_l$ for liquid and $\xi_v + \xi_a$ for gas, D the diffusivity, $\zeta = \xi_v / \beta g$ is the vapor fraction, $\mathbf{V}_k$ the velocity of the liquid, vapor and air with respect to the solid, $\mathbf{V} = \zeta \mathbf{V}_v + (1-\zeta)\mathbf{V}_a$ is the weighted velocity of the gas, and

$\mathbf{V}_{vg} = \mathbf{V}_v - \mathbf{V}_g$. The first sum is the dissipation due to the thermal effects, the second sum is the dissipation due to the moving liquid and gases, and the last term is the dissipation due to the relative movement of the vapor and air.

2.5. The final equations to be solved and the material laws

Substituting the free energies and dissipation function in the general constitutive relations and manipulating the equations, we obtain the final model that can be solved. The final variables of the system are molar volume fractions $\xi_s, \xi_l, \xi_v, \xi_a$, displacement $\mathbf{u}$, gaseous pressure $\hat{B}$, and temperature T. The evaporation rate of liquid $-\theta$ is used as an auxiliary variable. This strategy is adopted from Numerola with minor changes. The final system to be solved is

$$\xi_s + \xi_l + \xi_v + \xi_a = 1$$

$$\frac{\partial \rho_s}{\partial t} + \nabla \cdot (\rho_s \mathbf{U}_s) = 0$$

$$\frac{\partial \rho_l}{\partial t} + \nabla \cdot (\rho_l \mathbf{U}_l) = \theta_l$$

$$\frac{\partial \rho_v}{\partial t} + \nabla \cdot (\rho_v \mathbf{U}_v) = -\theta_l$$

$$\frac{\partial \rho_a}{\partial t} + \nabla \cdot (\rho_l \mathbf{U}_a) = 0$$

$$-\nabla \cdot \sigma - \rho_s \mathbf{g} = 0$$

$$(\rho c)_{\text{eff}} \frac{\partial T}{\partial t} - (e_v - e_l)\theta_l - \nabla \cdot (\lambda \nabla T) = 0$$

$$\ln \frac{\zeta \hat{B}}{(\zeta \hat{B})_0} =$$

$$= \frac{M_v}{RT}\left[L \frac{T - T_0}{T_0} + (c_v^p - c_l^p)Tln\frac{T}{T_0} + \frac{\hat{B} - \hat{B}_0}{\tilde{\rho}_l} \right]$$

$$+ \frac{\partial(\xi_l f)}{\partial \xi_l} +$$

$$+\frac{M_{\mathrm{v}}}{\tilde{\rho}_{\mathrm{l}}RT}\left[\xi_{\mathrm{s}}\frac{\partial f_{\Pi}}{\partial\xi_{\mathrm{l}}}\hat{B}_0\mathrm{tr}\epsilon+\frac{1}{2}\xi_{\mathrm{s}}\frac{\partial K}{\partial\xi_{\mathrm{l}}}(\mathrm{tr}\epsilon)^2\right].$$

with constraints

$$\xi_{\mathrm{k}}\geq 0 \text{ for k=s,l,v,a}.$$

The last equation is a generalized version of Clausius-Clapeyron equation which is obtained from the general constitutive equations. In the above equations system, the stress-strain relation is

$$\sigma=2\xi_{\mathrm{s}}G\epsilon^D-(\hat{B}-\xi_{\mathrm{s}}K\mathrm{tr}\epsilon-\xi_{\mathrm{s}}f_{\Pi}\hat{B}_0)\mathbf{I}$$

and the gaseous phase state equation is

$$\hat{B}=\tilde{\rho}_{\mathrm{k}}\frac{RT}{M_{\mathrm{k}}} \text{ for } k\in\{\mathrm{a,v}\}.$$

The modified Darcy's law for liquid water, water vapor and air are

$$\rho_{\mathrm{l}}\mathbf{U}_{\mathrm{l}}=-\tilde{\rho}_{\mathrm{l}}\frac{k_{\mathrm{l}}}{\mu_{\mathrm{l}}}\left[\nabla\hat{B}-\tilde{\rho}_{\mathrm{l}}\mathbf{g}+\tilde{\rho}_{\mathrm{l}}\frac{RT}{M_{\mathrm{v}}}\nabla\left(\frac{\partial(\xi_{\mathrm{l}}f)}{\partial\xi_{\mathrm{l}}}\right)\right.$$
$$+\rho_{\mathrm{l}}\frac{R}{M_{\mathrm{v}}}\frac{\partial f}{\partial\xi_{\mathrm{l}}}\nabla T+\xi_{\mathrm{s}}\frac{\partial f_{\Pi}}{\partial\xi_{\mathrm{l}}}\hat{B}_0\nabla(\mathrm{tr}\epsilon)$$
$$\left.+\hat{B}_0\mathrm{tr}\epsilon\nabla\left(\xi_{\mathrm{s}}\frac{\partial f_{\Pi}}{\partial\xi_{\mathrm{l}}}\right)\right]+\rho_{\mathrm{l}}\mathbf{U}_{\mathrm{s}}$$

$$\rho_{\mathrm{v}}\mathbf{U}_{\mathrm{v}}=-\tilde{\rho}_{\mathrm{v}}(\xi_{\mathrm{v}}+\xi_{\mathrm{a}})D\nabla\zeta-\zeta\tilde{\rho}_{\mathrm{v}}\frac{k_g}{\mu_g}\nabla\hat{B}+\rho_{\mathrm{v}}\mathbf{U}_{\mathrm{s}}$$

$$\rho_{\mathrm{a}}\mathbf{U}_{\mathrm{a}}=-\tilde{\rho}_{\mathrm{a}}(\xi_{\mathrm{v}}+\xi_{\mathrm{a}})D\nabla\zeta-(1-\zeta)\tilde{\rho}_{\mathrm{a}}\frac{k_g}{\mu_g}\nabla\hat{B}$$
$$+\rho_{\mathrm{a}}\mathbf{U}_{\mathrm{s}}$$

where the effects of gravity on gas and the direct solid deformation effects on liquid are neglected. Fourier's law for heat conductions is

$$\mathbf{q}=-\lambda\nabla T$$

and the internal energy difference in the energy balance equation is

$$e_{\mathrm{v}}-e_{\mathrm{l}}=l_0+(c_{\mathrm{v}}^p-c_{\mathrm{l}}^p)(T-T_0)-RT/M_{\mathrm{v}}.$$

Adsorption and swelling functions are

$$f=\begin{cases}a_1\left(\frac{\xi_s}{\xi_l}-\left(\frac{\xi_s}{\xi_l}\right)_0\right)^{a_2} & \text{for } \frac{\xi_s}{\xi_l}\leq\left(\frac{\xi_s}{\xi_l}\right)_0\\ \\ 0 & \text{for } \frac{\xi_s}{\xi_l}>\left(\frac{\xi_s}{\xi_l}\right)_0\end{cases}$$

$$f_{\Pi}=a_3\left(\frac{\xi_{\mathrm{s}}}{xi_{\mathrm{l}}}\right)^2+a_4\left(\frac{\xi_{\mathrm{s}}}{xi_{\mathrm{l}}}\right)+a5.$$

The adsorption function has been chosen so that it increases upon drying and decreases upon wetting in a way that adsorption and suction interactions vanish in fully saturated bentonite. This means that water is attached firmer to the solid skeleton of dry bentonite than to the skeleton of wet bentonite. The swelling function has been chosen such that the swelling interaction decreases upon wetting and vanishes at the fully swollen state. This, again, means that the solid skeleton in dry bentonite can store more "swelling" energy per volume change than the solid skeleton in wet bentonite. In a non-confined space this energy makes the solid volume to increase and in confined space it develops a swelling stress.

The mechanical parameters are

$$K=K_{\mathrm{init}}\left(\frac{\xi_{\mathrm{s}}/\xi_{\mathrm{l}}}{(\xi_{\mathrm{s}}/\xi_{\mathrm{l}})_{\mathrm{init}}}\right)^b$$

$$E=3(1-2\nu)K$$

$$G=E/(2(1+\nu)).$$

The hydraulic parameters are

$$k_j=k_{j,\mathrm{rel}}k_{\mathrm{sat}}$$

$$k_{\mathrm{l,rel}}=\xi^n$$

$$k_{\mathrm{g,rel}}\approx\text{constant}$$

$$\mu_l = 2.1 \cdot 10^{-6} \, \frac{\text{kg}}{\text{sm}} \, e^{\frac{1808.5 \, \text{K}}{T}}$$

$$\mu_l = 1.48 \cdot 10^{-6} \, \frac{\text{kg}}{\text{sm}} \, \frac{\sqrt{T/1\text{K}}}{1 + (119.4\text{K})/T}$$

$$D = D_{\text{ref}} \left(\frac{T}{T_{\text{ref}}} \right)^{\alpha}.$$

Finally, the thermal parameters for Febex bentonite are [3]

$$c_s^v = 1.38 \, \frac{\text{J}}{\text{kgK}^2} (T - 273.15\text{K}) + 732.5 \, \frac{\text{J}}{\text{kgK}}$$

$$\lambda = \lambda_{\text{sat}} + (\lambda_{\text{dry}} - \lambda_{\text{sat}}) / (1 + e^{(\chi - \chi')/dx})$$

$$(\rho c)_{\text{eff}} \approx \rho_l c_l^v + \rho_{\text{dry}} c_s^v,$$

where $\chi = \xi_l / (1 - \chi_s)$. We advise interested reader to see [3] for details, initial values, and values at the reference state.

3. Use of COMSOL Multiphysics

The model has been implemented with COMSOL Multiphysics 4.0a. Structural mechanics module with basic solid mechanics mode is used for the momentum balance equation. The modified glide and shear moduli are used instead of normal constant values. The effect of $\hat{B}$ and the swelling function has been implemented by using a weak contribution. The rest of the equations are implemented by using PDE interfaces mode with General Form PDE of the Mathematics package.

The implementation of the model is at test state, thereby no final solutions strategy or solver choice can be given here. For now, we solve the liquid, air and vapor mass balance equations together with the energy balance equations and Clausius-Clapeyron equation as fully coupled problem. Then the momentum balance and mass balance for the solid are solved separately. This strategy is adopted with minor changes from the implementation of the CSC – IT Center for Science [3].

The time-dependent solver that we use for now is the order one BDF, that is, the implicit Euler. Nonlinear solver is used with a high number of iterations which allows us to use relatively long time-steps. This strategy has been adopted from Numerola's implementation. Linear systems are solved with MUMPS.

The indicator functions in the free energies should automatically keep the system within the limits that the restrictions on the molar volume fractions give. At some points of the equation manipulation, however, the indicator functions are neglected. Therefore, constraints on the molar volume fractions may have to be used in the numerical implementation. A problem with this approach is that the constraints generate constraint forces that are not necessarily the intended ones. Thereby, we may alternatively use smoothed indicator functions that are carried through the equation manipulations to the final equation system in the future. These indicator functions would act as one sort of physical penalty functions.

4. Discussion

The model presented here is one approach to model the saturation of compacted bentonite. The model concentrates on the thermo-hydraulic behavior of compacted bentonite on macro level which means that the model leaves some questions open of the behavior of the compacted bentonite. One such question is related to the hydraulic parameters used in the model. The porous space of bentonite is divided into interlaminar porous space and free porous space, both of which have been covered by a single porosity in the model. Therefore, the model here cannot take into account the dependency of hydraulic parameters on the water content in these different pore types. These effects are incorporated in the model only by using a hydraulic permeability fitted into experimental results which means that new fit has to be produced if anything changes in the modeled case.

In general, no chemical effects are included in the model. The behavior of bentonite, however, strongly depends on the chemical composition of the intruding water and on the type of interlaminar cations. Not taking these effects into account in the model directly simply means that they are present somehow in the

model parameters. Therefore, at least some of the model parameters have to be fitted separately for each water-bentonite combination. This feature weakens the prediction capability of the model.

The mechanical behavior and the swelling have been incorporated in the model by "crude approach" by the developer's words. Especially the dynamics of the mechanical behavior may need fine tuning. Moreover, the model does not take plastic behavior of bentonite into account although it has been observed experimentally in wetting test [3].

Despite the fact that the model does not include everything, it provides a means to add new features. Further, the procedure used in deriving the final equations of the model may be used to develop virtually any kinds of thermodynamically sensible models.

5. References

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