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BACK ANALYSIS OF A COUPLED THERMO-HYDRO-MECHANICAL MODEL BASED ON INSTRUMENTED CONSTANT VOLUME COLUMN TEST

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Abstract. This study contributes to identification of the constitutive model parameters for coupled THM models for unsaturated sand-bentonite mixtures via back analysis approach. The approach strategy consists of: definition of the forward model, sensitivity analysis, selection of optimization algorithm, selection of a set of parameters to be optimized, setup of the parameter's constraints, and assessing the reliability and accuracy of the identified model and material parameters. For this analysis the iterative direct approach based on numerical solution of the direct problem and minimization of an objective function has been selected. It is given an example of application of the selected inverse analysis procedure to identification of parameters involved in a modified Barcelona Basic Model taking into account of variation of temperature.

1 INTRODUCTION

Current solution for the radioactive waste disposal is to place the canisters containing the waste in a tunnel system located deep in the host rock. The canisters are surrounded by expansive clay that composes the buffer. The behavior of the buffer needs to be well understood in order to guarantee the safety and the efficiency of the radioactive waste repository. The clay in the buffer, initially unsaturated, is subjected to high temperature emitted by the radioactive waste and to hydraulic gradients induced by water permeating from the host rock. As a consequence swelling and shrinking phenomena take place with the variation of water content and temperature.

During the past decade a number of numerical simulations were carried out in order to assess the physical processes and predict the behavior of the buffer soil in a real environment. Because the coupled THM phenomena are complicated the constitutive models were gradually gaining complexity. This material model complexity often invokes the need of large sets of model parameters that are not simple for determining experimentally. Several researchers contributed with their experimental studies for deriving unsaturated soil models parameters. Particularly for the Barcelona Basic Model (BBM), contributions are made by e.g. Lloret et al [8] for FEBEX bentonite, Geiser et al [5] for sandy silt, Agus [1] for sand-bentonite mixtures. However due to device and sensor restrictions it may not be always possible directly to measure and provide sufficient and reliable laboratory test data for determining the material model parameters, especially, the parameters with the effect of temperature. The available experimental data may request back analysis procedure for identification of model parameters by minimizing the error function between measurement and e.g. numerical simulation results. For instance, Schanz et al (2008) [11] determined couple hydro-mechanical parameters for the modified BBM model [4] from measurement in swelling pressure cell. In the present paper, the back analysis procedure is introduced to identify the coupled THM model parameters for sand-bentonite mixture based on constant volume column test data. The approach strategy consists of: definition of the forward model, sensitivity analysis, selection of optimization algorithm, selection of a set of parameters to be optimized, setup of the parameter's constraints, and assessing the reliability and accuracy of the identified model parameters.

2 CONSTITUTIVE EQUATIONS OF THE COUPLED THM MODEL

Following the two stress variable concept in unsaturated soil mechanics, the elastic part of the strain increment is taken to be a sum of the increments of suction induced $\boldsymbol{\varepsilon}^{s-e}$, net stress induced $\boldsymbol{\varepsilon}^{\sigma-e}$ and the strain increment due to temperature change $d\boldsymbol{\varepsilon}^{T-e}$. The final relation for the elastic strain increment reads:

$$d\boldsymbol{\varepsilon}^{e} = d\boldsymbol{\varepsilon}^{\sigma-e} + d\boldsymbol{\varepsilon}^{s-e} + d\boldsymbol{\varepsilon}^{T-e} \tag{1}$$

The nonlinear elastic law for the volumetric strain induced by the net stress is expressed in Eq. 2.

$$d\varepsilon_v^{\sigma-e} = \frac{\kappa_i(s)}{1+e}\,\frac{dp'}{p'} \quad \text{and} \quad p' = p - \max(p_g, p_l) \tag{2}$$

$$\kappa_i(s) = \begin{cases} \kappa_{io}\,(1+\alpha_i\, s) & \text{if } 1+\alpha_i\, s \geq 0.001 \\ 0.001\, k_{io} & \text{if } 1+\alpha_i\, s < 0.001 \end{cases} \tag{3}$$

where p is mean total stress, p' is the mean net stress in unsaturated state or effective stress in saturated state, p_g and p_l are gas pressure and liquid pressure, e is the void ratio,

κ_{io} and α_i are model parameters. For deviatoric elastic strains, a constant Poisson's ratio is used.

Suction and temperature induce only volumetric strains with constitutive equations given as following:

$$d\varepsilon_v^{s-e} = \frac{\kappa_s(p', s)}{1+e}\frac{ds}{s+p_{at}} \quad ; \quad d\varepsilon_v^{T-e} = \alpha_o\, dT \tag{4}$$

with

$$\kappa_s(p', s) = \kappa_{so}\kappa_{sp}\ \exp\left(\alpha_{ss}\, s\right) \tag{5}$$

and

$$\kappa_{sp} = \begin{cases} 1 + \alpha_{sp}\ln\left(\frac{10^{-20}}{p_{ref}}\right) & \text{if } p' \leq 10^{-20} \\ 0 & \text{if } p' \geq p_{ref}\exp\left(\frac{-1}{\alpha_{sp}}\right) \\ 1 + \alpha_{sp}\ln\left(\frac{p'}{p_{ref}}\right) & \text{elsewhere} \end{cases} \tag{6}$$

The parameters involved are: α_o for the elastic thermal strain; κ_{so} is the elastic stiffness parameter in changing of suction at zero net stress; p_{at} is the atmospheric pressure; α_{ss} and α_{sp} are model parameters. The elastic modules κ_i and κ_s may be considered not dependent on temperature in case of moderate temperature gradients.

The yield surface in BBM model is given in the deviatoric plane $q-p$ via the following equation:

$$F = q^2 - M^2\left(p' + p_s\right)\left(p_o - p'\right) = 0 \tag{7}$$

where $q = \sqrt{\frac{3}{2}\boldsymbol{\sigma}^D : \boldsymbol{\sigma}^D}$, with deviatoric stress defined as $\boldsymbol{\sigma}^D = \boldsymbol{\sigma'} - \frac{1}{3}\boldsymbol{\sigma'} : \boldsymbol{I}$. The preconsolidation pressure p_o depends on suction and according to Alonso (1990) [2] it is defined as:

$$p_o = p^c\left(\frac{p_o^*}{p^c}\right)^{\frac{\lambda(0)-\kappa_{io}}{\lambda(s)-\kappa_{io}}} \tag{8}$$

where p^c is a reference pressure, p_o^* is the preconsolidation pressure for a saturated state, $\lambda(0)$ is a plastic stiffness parameters for changes in effective stress at saturated state. The stiffness parameter for changes in the mean net stress at given suction is defined by:

$$\lambda\left(s\right) = \lambda\left(0\right)\left[\left(1-r\right)\exp\left(-\beta s\right) + r\right] \tag{9}$$

where r and β are model parameters.

The tensile strength p_s, follows a linear relationship with suction and is a function of temperature:

$$p_s = p_{s0} + k\, s \exp(-\rho \Delta T) \quad \text{and} \quad \Delta T = T - T_{ref} \tag{10}$$

where k is parameter that takes into account the increase of tensile strength due to suction, p_{s0} is tensile strength in saturated state, ρ is a parameter that takes into account the decrease of the tensile strength due to temperature increase, T_{ref} is a reference temperature.
The isotropic hardening depends on the plastic volumetric strain according to:

$$dp_o^* = \frac{1+e}{\lambda(0) - \kappa_{io}}\, p_o^*\, d\varepsilon_v^p \tag{11}$$

For hydraulic process, advective flow of the water phase is described by the generalized Darcy's law:

$$\boldsymbol{q}_l = -\frac{\boldsymbol{k} k_{rl}}{\mu_l} \left(\nabla p_l - \rho_l \boldsymbol{g}\right) \tag{12}$$

where μ_l is the dynamic viscosity of the pore liquid, $\boldsymbol{g}$ is the gravity acceleration, ρ_l is the liquid density. The tensor of intrinsic permeability $\boldsymbol{k}$, is supposed to depend on porosity according to the Kozeny's model:

$$\boldsymbol{k} = \boldsymbol{k}_o \frac{\phi^3}{(1-\phi)^2} \frac{(1-\phi_o)^2}{\phi_o^3} \tag{13}$$

where ϕ is the porosity, ϕ_o is a reference porosity, $\boldsymbol{k}_o$ is the intrinsic permeability for matrix with porosity ϕ_o. The relative permeability k_{rl}, is derived from Mualem-van Genuchten closed form model, [7]:

$$k_{rl} = \sqrt{S_e}\left(1 - \left(1 - S_e^{1/\lambda}\right)^{\lambda}\right)^2 \tag{14}$$

where λ is a shape parameter for retention curve and S_e is defined as:

$$S_e = \frac{S_l - S_{rl}}{S_{ls} - S_{rl}} = \left(1 + \left(\frac{p_g - p_l}{P_0}\right)^{\frac{1}{1-\lambda}}\right)^{-\lambda} \tag{15}$$

where S_l, S_{ls} and S_{rl} are the current, the maximum and the residual liquid degree of saturation, P_0 is a model parameter.

Fick's law is adopted to define the diffusive flux of water vapour $\boldsymbol{i}^v$:

$$\boldsymbol{i}^v = -\left(\phi \rho_v\, S_l\, D_m \boldsymbol{I}\right) \nabla \omega^v \tag{16}$$

where ρ_v is the vapour density, ω^v is the mass fraction of the vapour, $\mathbf{I}$ is the identity matrix and D_m is the diffusion coefficient of vapour in m^2/s is defined by:

$$D_m = \tau D \frac{(273.15 + T)^n}{P_g} \tag{17}$$

where τ is the tortuosity, D is the molecular diffusion coefficient at temperature 273.15K and $P_g = 101$kPa, and n is a coefficient.
Fourier's law is adopted for heat conduction flux, $\boldsymbol{i}_c$, of heat:

$$\boldsymbol{i}_c = -\lambda_T \nabla T \quad \text{where} \quad \lambda_T = \lambda_{sat}^{S_l} \lambda_{dry}^{(1-S_l)} \tag{18}$$

where λ_T is the soil thermal conductivity, λ_{sat} and λ_{dry} are soil thermal conductivity at the saturated and dry state, respectively.

In summary, there are total 26 parameters to describe the behaviour of coupled THM model.

- Parameters involved in modelling net stress driven processes ($\mathrm{d}\boldsymbol{\sigma} \neq 0$):
  $\boldsymbol{\mathcal{M}} = \{\kappa_{io}, \alpha_i, p_{ref}, \lambda(0), r, \beta, k, p_{s0}, p^c, M, \alpha, e_o, p_o^*\}$
- Parameters involved in modelling suction driven processes ($\mathrm{d}s \neq 0$):
  $\boldsymbol{\mathcal{H}} = \{P_0, \lambda, \phi_0, \kappa_o, \kappa_{s0}, \alpha_{ss}, \alpha_{sp}\}$
- Parameters involved in modelling temperature driven processes ($\mathrm{d}T \neq 0$):
  $\boldsymbol{\mathcal{T}} = \{\tau, D, \lambda_{sat}, \lambda_{dry}, \alpha_0, \rho\}$

The total parameters are summarised in vector: $\boldsymbol{x} = \{\boldsymbol{\mathcal{H}}, \boldsymbol{\mathcal{T}}, \boldsymbol{\mathcal{M}}\}$

3 IDENTIFICATION OF CONSTITUTIVE PARAMETERS FOR COUPLED THM MODEL VIA BACK ANALYSIS

The back analysis approach strategy consists in the following steps: definition of the forward model, parameter sensitivity analysis; selection of a set of parameters to be optimized; selection of optimization algorithm; setup of the parameter constraints, and assessing the reliability and accuracy of the identified model parameters.

3.1 Sensitivity analysis

The influence of model parameters on the model response is determined based the following fundamental equations.

1- Determination of scaled sensitivity (SS): The *SS* analysis indicates the amount of information provided by the *i-th* type of observation for the estimation of *j-th* parameter. We define *SS* for each particular observation k of the *i-th* type of observation:

$$SS_{i,j}^k = \frac{x_j}{y_i^k} \frac{\partial y_i^k}{\partial x_j} \tag{19}$$

Thus we use k to denote different observations done during the experiment at different time, e.g. t_k, $k = 1...N$

2- Determination of composite over time scaled sensitivity (CSS): CSS is used to measure the *i-th* type of observation sensitivity to a given parameter x_j over the whole time of measurement:

$$CSS_{i,j} = \sqrt{\frac{1}{N} \sum_{k=1}^{N} \left(SS_{i,j}^{k} \right)^2} \tag{20}$$

3- Determination of sensitivity factor $\gamma_{i,j}$ for each of parameters: The sensitivity factor is used to normalise $CSS_{i,j}$ in the range from zero to one.

$$\gamma_{i,j} = \frac{CSS_{i,j}}{\max_j \{CSS_{i,j}\}} \tag{21}$$

In order to understand the response of the model in different time intervals, the sensitivity analysis later done for the THM model is performed for three different time intervals, namely at the end of the experiment ($T100$), at 50% of the total time of the experiment ($T50$), and at the first time step of calculation process, ($T0$). In our particular case the vector of model response is $\boldsymbol{y} = \{S_l(t), T(t), \sigma_{yy}(t)\}$.

3.2 Model–parameter optimization via direct inverse approach

The direct inverse approach, which consists of an automated iterative procedure correcting the trial values of the unknown parameters by minimizing an error function, is applied here for the back analysis of the instrumented constant volume column test. The optimization algorithm uses the simplex Nelder-Mead optimization method [10]. The objective function employed here is the absolute mean error F_{AM} (Eq. 22). The solution of the optimization problem is considered against one of following criteria: $F_{AM} \leq \epsilon$, the maximum number of iteration, or Eq. 23. The optimization routine is executed by means of the VARO^{2}PT [13] optimization tool.

$$F_{AM}(\boldsymbol{x}) = \frac{1}{n} \sum_{i=1}^{n} |y_i^{meas} - y_i(\boldsymbol{x})| \tag{22}$$

$$\Delta F_{AM} = |F_{AM} - F_{AM}^{prev}| \leq \Delta_\epsilon \tag{23}$$

where $\boldsymbol{y}^{meas}$ and $\boldsymbol{y}$ are the vectors of the measurement and numerical (model) observations, F_{AM}^{prev} is the value of the objective function from the previous step, ϵ and Δ_ϵ are critical values to stop the optimization iterations.

3.3 Assessment of the quality of the optimal set of model parameters

The values of the sensitivity factors $\gamma_{i,j}$ are used to assess the reliability of optimal set of parameters. The mean value ν_j gives the overall model sensitivity to $j-th$ parameter:

$$\nu_j = \frac{1}{n}\sum_{i}^{n}\gamma_{i,j} \tag{24}$$

3.4 Assessment of the goodness of the fit

We may use several strategies to back calculate the model parameters and depending on the strategy we may obtain different optimal parameter sets. In order to compare different solutions and assess the goodness of the fit we calculate the following statistical measures: the mean error, the standard deviation and skewness, defined as:

$$\mu = \frac{1}{n}\sum_{i=1}^{n}\varepsilon_i \quad ; \quad \sigma = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(\varepsilon_i-\mu)^2} \quad ; \quad \gamma_1 = \frac{\mu_3}{\sigma^3} \tag{25}$$

where n is a number of measured samples and ε_i is the error between $i-th$ measurement and simulation values, μ_3 is the third moment about the mean.

4 DEFINITION OF THE FORWARD PROBLEM

A series of hydration test and heating test were performed in the newly developed THM apparatus, [9]. The experimental data obtained is used for back analysis and the boundary and initial conditions of the tests are used in building the model for the forward calculation.

4.1 Hydration test

During the hydration test we measured the water absorbed by sand-bentonite mixture (SBM) and the vertical stress. The sample was hydrated from the top and development of swelling pressure with time was measured at top and bottom ends of the sample. The evolution of water front along the vertical axis of specimen is recorded by three Time Domain Reflectometry (TDR) sensors.

For numerical simulation of hydration test, the numerical model is built in the X-Y plane, Fig. 1a. At the top and the bottom of the model liquid flux boundary condition is applied. The distances from points 1, 2, 3 to the top of the model are 50 mm, 150 mm, 250 mm, respectively (see Fig. 1). Points 1, 2 and 3 correspond to the position of the measurement devices. Point 4 is located at the bottom of the sample where the load cell measurements are recorded.

4.2 Heating test

The heating test series was carried out to investigate the behavior of SBM sample by heating. The temperature boundary conditions is a prescribed temperature at the bottom

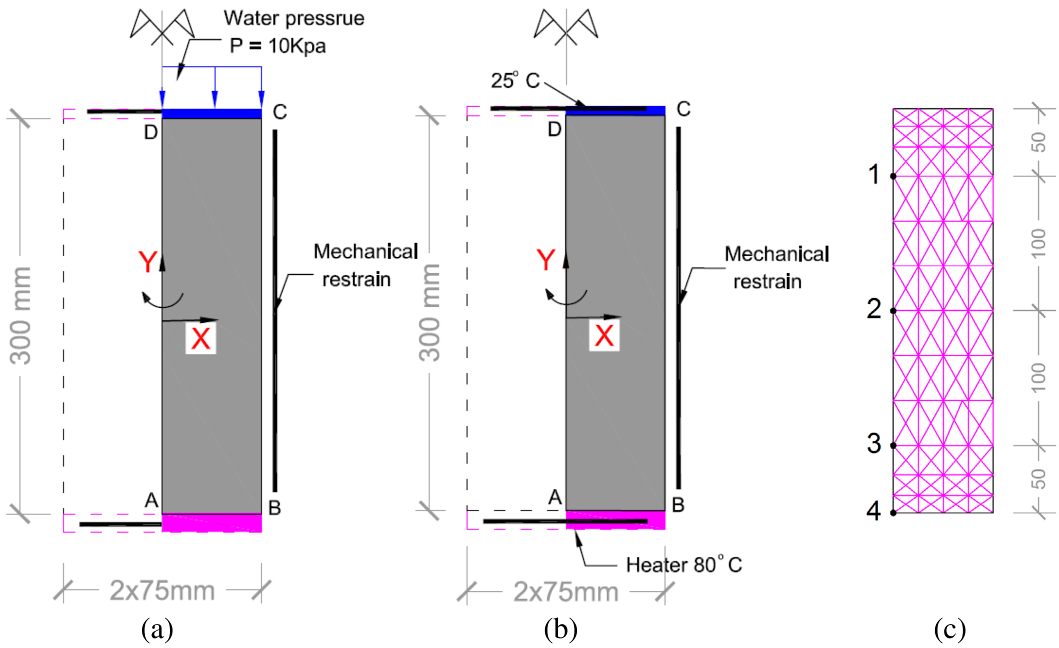

Figure 1: Numerical model: (a)– Hydration test model; (b)– Heating test model; (c)– FE-discretization with the observation points

(80 ^{o}C) and at the bottom (25 ^{o}C) and zero heat flux at the lateral boundaries (see Fig.1b). The change of humidity was measured by the RH sensors, temperature sensors are also installed at the same place where RH sensors are located. Water content within the specimen is measured by TDR sensor inserted in the soil specimen and thermocouple sensors are placed nearby to the TDRs to measure the current local temperature. No water is supplied. The independent variables for the model are displacement vector $\boldsymbol{u}$, liquid pressure p_l and temperature T.

5 RESULTS AND DISCUSSION

5.1 Results of the sensitivity analysis

For the hydration test model, the material response is characterised in the terms of degree of saturation (S_l) and vertical stress (σ_{yy}). The vector of model parameters is now $\boldsymbol{x}^H = \{\boldsymbol{\mathcal{H}}, \boldsymbol{\mathcal{M}}\}$ and the vector of model response is $\boldsymbol{y} = \{S_l(t), \sigma_{yy}(t)\}$. The results of the sensitivity analysis are presented in Fig. 2. No data is presented for the parameters that have very low influence to the model responses.

For the heating test model, the vector of model parameters is $\boldsymbol{x}^T = \{\boldsymbol{\mathcal{H}}, \boldsymbol{\mathcal{T}}, \boldsymbol{\mathcal{M}}\}$ and the vector of the model response is $\boldsymbol{y} = \{S_l(t), \sigma_{yy}(t), T(t)\}$. The results of sensitivity analysis are presented in Fig. 3. The analysis of temperature response indicates that λ_{sat} is the parameter influencing the most the heat conduction process. The analysis of

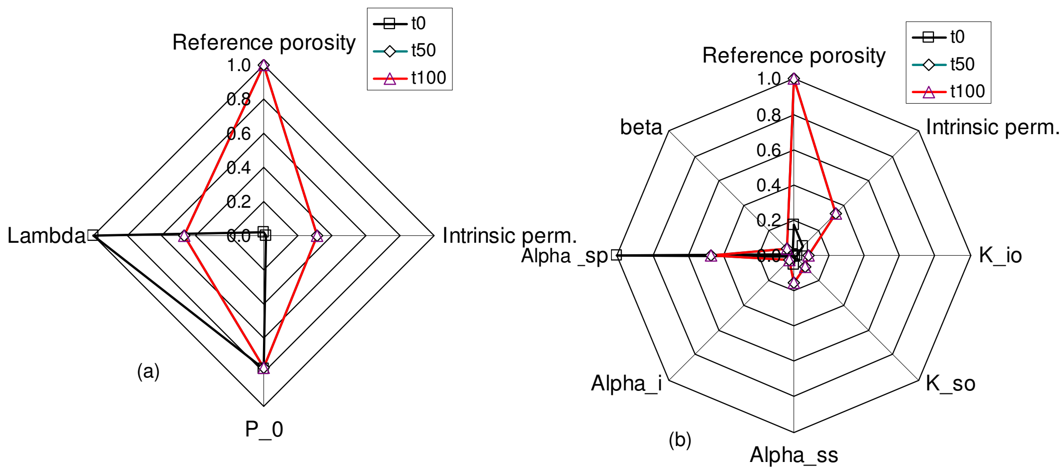

Figure 2: Hydration test: (a)– γ_j of degree of saturation. (b)– γ_j of vertical stress

the vertical stress indicates that the parameter α_{sp} is significantly influencing the model response at the beginning of the test and its influence is reduced with time. Beside that, the parameter $\boldsymbol{k}_o$ is significantly influencing the vertical stress evolution.

5.2 Results of the optimization

For the initial forward calculation we used parameter set with parameter values found in literature. The mechanical parameters ($\boldsymbol{\mathcal{M}}$) are taken from [1]. The values of thermal conductivity λ_{sat} and λ_{dry} are used as for the FEBEX bentonite reported in [12]. The value for the molecular diffusion coefficient of vapour in the air is taken from [6]. The parameters for the retention curve (Eq. 15) are obtained via regression analysis from test on SBM [3].

Figure 4 presents the comparison between the calculated and measured S_l in the hydration test before and after optimization based on the data from only this test. Fig. 5(a) presents the evolution of the temperature and S_l obtained using the initial model parameter set. Fig. 5(b) depicts the model response after the parameter set optimization using only data from this test.

There are two types of tests to calibrate the coupled THM properties of SBM. When consider the boundary conditions during our tests it can be concluded that there are four possible strategies for identification of the model parameters: (1) to identify the $\boldsymbol{\mathcal{H}}$ and $\boldsymbol{\mathcal{M}}$ parameters using solely the hydration test back analysis; (2) to identify $\boldsymbol{\mathcal{H}}$, $\boldsymbol{\mathcal{M}}$ and $\boldsymbol{\mathcal{T}}$ parameters via back analysis base of solely the heating test; (3) to identify $\boldsymbol{\mathcal{T}}$ model parameters based on heating test when using $\boldsymbol{\mathcal{H}}$ and $\boldsymbol{\mathcal{M}}$ calibrated via (1); and (4) to identify $\boldsymbol{\mathcal{M}}$ model parameters in hydration test based on $\boldsymbol{\mathcal{H}}$ obtained by inverse modelling of the heating test. The results of the application of these four strategies are given in the Table 3.

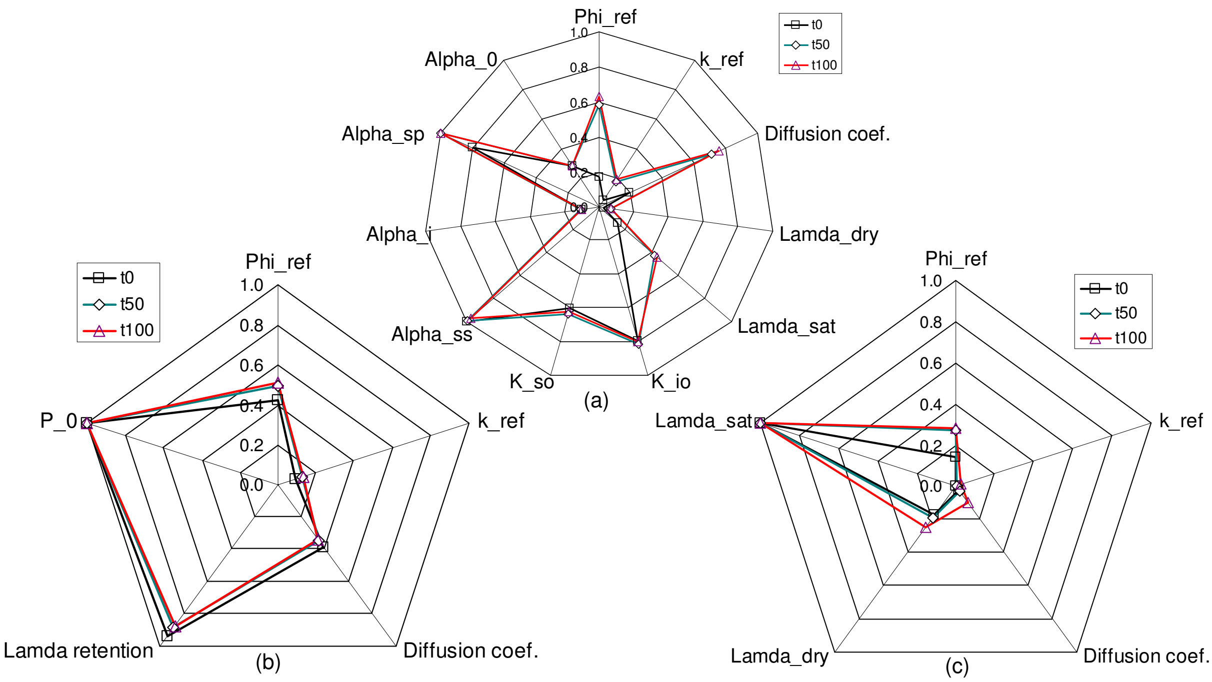

Figure 3: Heating test: (a)– γ_j of vertical stress (σ_{yy}). (b)– γ_j of degree of saturation. (c)– γ_j of temperature

5.3 Assessment of the quality of the optimized parameters

Table 1 presents the assessment of the quality of the identified parameters. The results show that P_0 in hydraulic equation and α_{sp} have a strong influence on the model response. Therefore these two parameters are calibrated most reliably.

5.4 Assessment of the goodness of the fit

In order to assess the goodness of the fit in each result after optimization, residual analysis method is adopted. The mean value, standard deviation and skewness are computed to assess the normality of the residuals.

Table 2 presents the result of the residual analysis. The results indicated that the optimization of hydration test obtained the best fit between measurement and numerical simulation.

6 CONCLUSION

The paper presents the strategy to identify the parameters for coupled THM model of sand bentonite mixture (SBM). Direct back analysis to two types of experiments is applied to identify the model parameters to which the model response is the most sensitive. Further, the quality of the obtained optimal set of parameters is assessed. One may expect

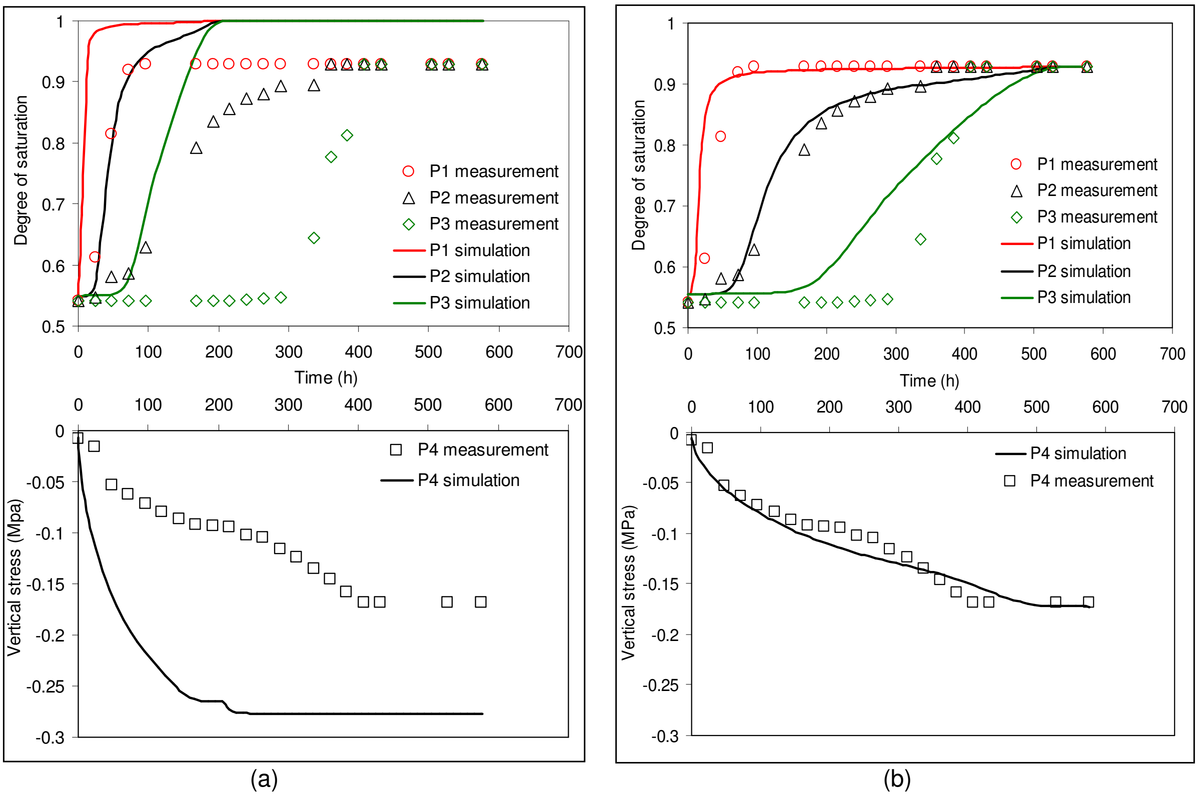

Figure 4: Hydration test–simulation vs. measurement: (a) Before optimization, (b) After optimization

that the best model calibration can be obtained combining the hydration and the heating test data, however the result of out investigation show that the independent back analysis of the heating test provides the best and most reliable set of model parameters.

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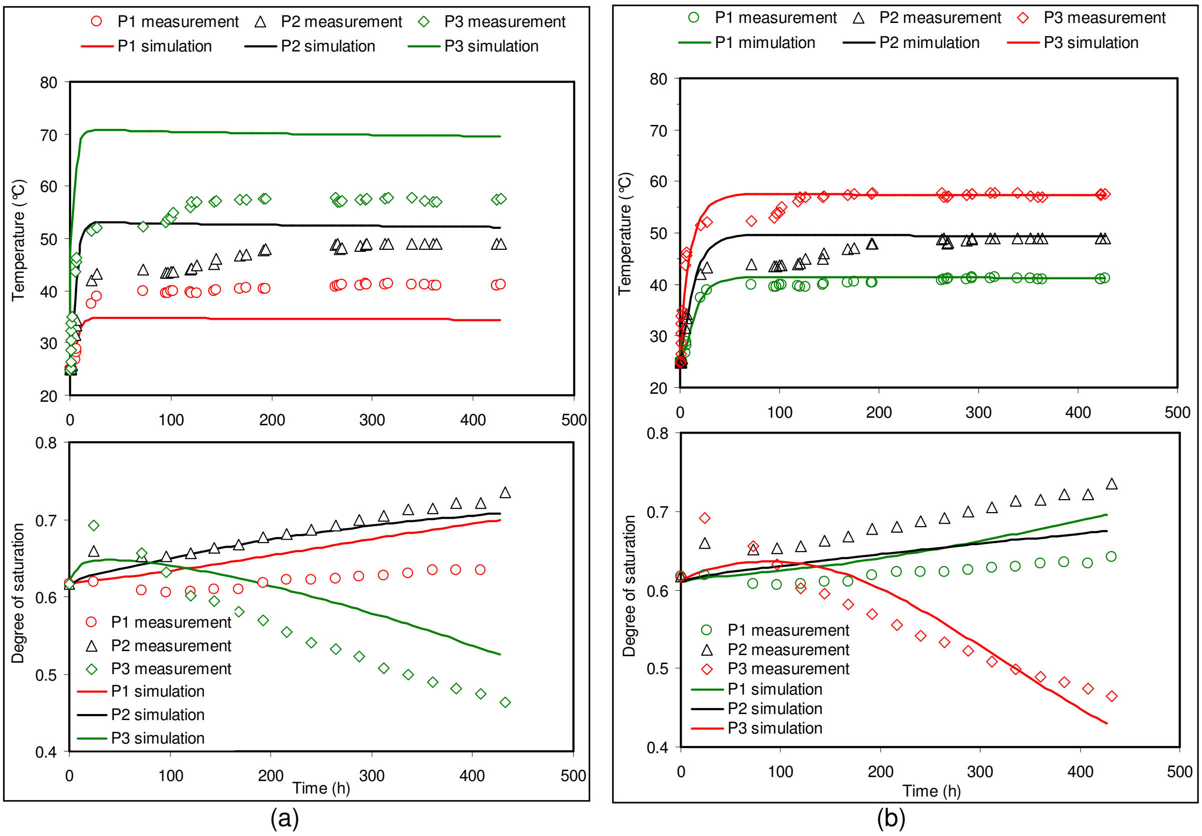

Figure 5: Heating test–simulation vs. measurement: (a) Before optimization, (b) After optimization

Table 1: The quality of the optimized parameters

$\{y_i\}$	$\{x_j\}$										
	k_{io}	k_{so}	α_{ss}	α_i	α_{sp}	P_0	λ	k_o	D	λ_{dry}	λ_{sat}
THM:											
S_l	0.000	0.000	0.000	0.000	0.000	1.000	0.895	0.118	0.355	0.000	0.000
T	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.014	0.059	0.214	1.000
σ_{yy}	0.810	0.623	1.000	0.103	0.911	0.000	0.000	0.116	0.478	0.046	0.291
HM:											
S_l	0.000	0.000	0.000	0.000	0.000	1.000	0.828	0.271	0.000	0.000	0.000
σ_{yy}	0.100	0.099	0.182	0.035	1.000	0.000	0.000	0.392	0.000	0.000	0.000
ν	0.182	0.144	0.236	0.028	**0.382**	**0.400**	**0.345**	0.182	0.178	0.052	0.258

Table 2: Residual analysis for the back analyzes

	Hydration	Heating	Heating →Hydrat.	Hydrat. →Heating
Mean value	-0.0035	0.0127	0.0216	0.00785
Standard deviation	0.0704	0.0400	0.0837	0.04140
Skewness	0.0498	0.0793	0.5108	-0.13469

Table 3: Summary of the parameters before and after back analysis

Par.	Unit	Initial	Constrain Min.	Constrain Max.	Hydrat.	Heating	Heating => Hydration	Hydrat. => Heating
TEP Elastic Parameters								
k_{io}	-	0.0029	0.0019	0.0039	0.0033	0.0029	0.0037	0.0033
k_{so}	-	0.1426	0.1	0.2	0.1468	0.1426	0.181	0.1468
a_{ss}	-	-0.1128	-0.09	-0.18	-0.103	-0.1128	-0.141	-0.103
a_i	-	-0.006	-0.003	-0.009	-0.0063	-0.006	-0.0069	-0.0063
a_{sp}	-	-0.3	-0.15	-0.50	-0.333	-0.3	-0.327	-0.333
Hydraulic and thermal parameters								
P_0	MPa	15	7.00	25.00	16.35	15	19.73	16.35
λ	-	0.53	0.40	0.80	0.564	0.543	0.543	0.564
k_o	(m^2)	2.07E-19	5.0E-22	1.00E-18	5.62E-20	3.59E-21	3.59E-21	5.62E-20
D	(*)	5.90E-06	1.0E-06	1.00E-05	5.90E-06	6.36E-06	6.36E-06	6.10E-06
τ	-	0.8	0.70	1.10	0.8	0.79	0.79	0.83
n	-	2.3	1.50	3.00	2.3	2.5	2.5	2.48
λ_{sat}	-	1.507	1.20	1.80	1.507	1.749	1.749	1.560
λ_{dry}	-	1.00	0.70	1.20	1.00	1.18	1.18	1.00

(*) : $m^2 s^{-1} K^{-n} Pa$

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