NUMERICAL SIMULATION AND BACK ANALYSIS OF COUPLED THERMO-HYDRO-MECHANICAL BEHAVIOR OF SAND-BENTONITE MIXTURE

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Abstract. *This paper is aimed mainly to study in terms of numerical simulation the coupled THM processes in engineered barrier and sealing systems designed for the isolation of radioactive waste. The THM experiments are performed in the Soil Mechanics Laboratory-Bauhaus University Weimar. The finite element code Code-Bright (UPC) is used for numerical solution of the considered THM coupled problems. The performed experiments are numerically simulated in order to reveal the influence of the temperature and hydraulic gradients on the distribution of temperature, mechanical stress and water content. The following tests are simulated:*

1- *Swelling test: Water is supplied to sand-bentonite mixture sample from the top and the measurements are done during the wetting process.*

2- *THM test: Soil sample is heated from below to 80° C. The features of the THM behavior are recorded.*

Sensitivity analysis is carried out to identify the parameters which influence the most the response of the numerical models. Results of back analyses of the model parameters are reported and critically assessed.

1 INTRODUCTION

Recently, the utilization of some types of clay for the isolation of nuclear waste materials underlies many research works. High radioactive substance might permeate with water or brine though barrier systems to biosphere. The temperature emitted from nuclear waste canisters also requests the study of temperature effect in soils. The water absorbed from the host rock may induce swelling phenomenon which can yield to a damage of the nuclear waste containers. All the above phenomena need to be well understood in order to guarantee for the safety and the efficiency of the waste sealing construction.

Understanding and proper modeling of such phenomena as heat transfer, water flow, and stress changes in the engineered clay barrier and their influence on the barrier properties are important issues in performance assessment of the nuclear waste repositories. Olivela [10], Loret [6], and Agus [1], have contributed their experimental study to such kind of problems.

Although experimental works play an important role in studying of buffer and sealing systems behaviour, they are often time consuming and costly. That is why numerical modelling is of essential importance for prediction of engineered barrier system behaviour not only during a particular experiment but also continuously in a period of thousands years for which experimental work can not be performed.

Code_Bright finite element program is used in this work for the study of THM behaviour of clay in terms of numerical simulations. The Code_Bright, with its coupled THM formulations, has been widely used in design and performance assessment studies of nuclear waste disposal (Olivella [11] ; Gens [5]; Alonso [3]). Corresponding to the two laboratory tests considered in the present study, we performed two types of numerical simulations: coupled Hydro-Mechanical (HM) behaviour and fully coupled THM numerical simulation.

The present paper addresses the sensitivity analysis and the identification procedure via back analysis of sand-bentonite mixture model parameters. Due to the large number of parameters involved in the THM coupled models we first performed a sensitivity analysis to identify the model parameters that influence the most the modelling results. The current study explores systematic approach to model sensitivity and back analysis in case of coupled THM problems.

2 DESCRIPTION OF THE TESTS

The newly developed THM apparatus, [7] is shown in *fig. 2.1*. The column is divided in three parts: top, bottom and cylindrical body. The top and the bottom have got the same arrangement. Arrangements are been done to place heater, load cell and hydration system at the top and the bottom. Cylindrical body can hold a sample of 300 mm in height and 150 mm in diameter. Water is supplied to the sample via burette. The soil sample is heated by heater installed below the sample. The TEFLON layer prevents heat dissipation to the surrounding environment. HM test data and THM test data obtained by using the above described equipment are compared with the numerical simulations. Protocols for HM and THM test are given in the following sections.
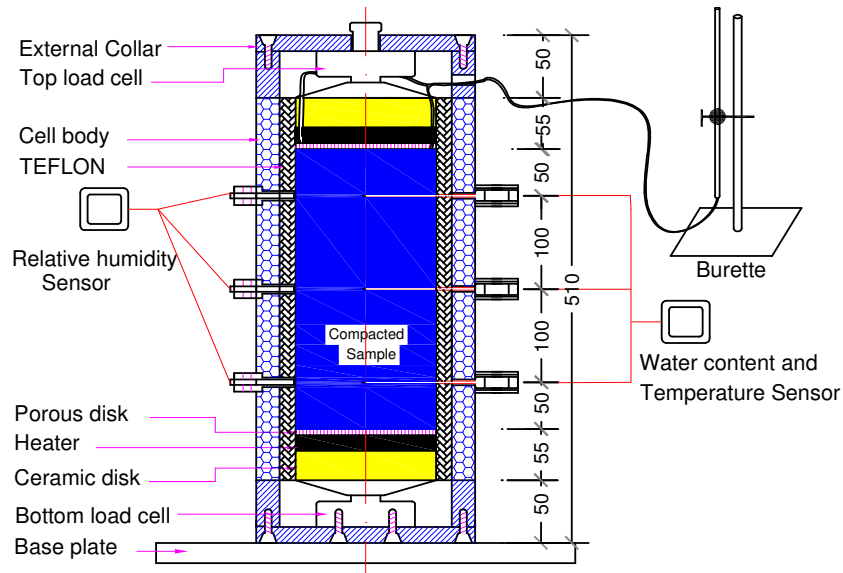
Fig. 2.1: THM apparatus in 2D view

2.1 HM test

In order to investigate the hydraulic permeability and mechanical behaviour of compacted sand-bentonite mixture, a hydro-mechanical swelling test was carried out. Water is supplied to the soil sample with water pressure $P_l = 10$ kPa from the top of sample by the burette. Heater does not work in this test. Load cells are installed on the top and the bottom of the specimen in order to measure the vertical stress due to swelling. Three relative humidity (RH) sensors are set along the soil sample to monitor the relative humidity/suction.

When water is absorbed into the soil sample, mechanical and chemical interactions occur which induce the swelling phenomena. Evolution of water content at the inside of specimen is measured by three water content sensors (TDR) which are located along the cylindrical column.

2.2 THM test

In order to investigate the change of water content and mechanical behaviour due to heating, a THM test was carried out [7]. In this test, no water is supplied. The soil specimen is heated from the bottom of the soil sample. A redistribution of the water content occurs due to heating. The change of humidity is also measured by the RH sensors, temperature sensors are also installed at the same place of RH sensors. Water content within the specimen is measured by TDR sensor penetrated in the soil specimen and temperature sensors placed nearby.

3   THEORETICAL FRAMEWORK

The equations that govern the THM simulation are the balance equations, the constitutive equations and the equilibrium restrictions.

3.1 Balance Equations

The following balance equations are used for THM numerical simulations [11].

3

Mass balance of water

Water is present in liquid an gas phases. The total mass balance of water is expressed as:

$$\frac{\partial}{\partial t}\left(\theta_l^w S_l \phi + \theta_g^w S_g \phi\right) + \nabla \cdot \left(\mathbf{j}_l^w + \mathbf{j}_g^w\right) = f^w \tag{2.1}$$

Where, f_w is an external supply of water. An internal production term is not included because the total mass balance inside the medium is performed.

Momentum balance for the medium

The momentum balance reduces to the equilibrium of stresses if the inertial terms are neglected:

$$\nabla \cdot \boldsymbol{\sigma} + \mathbf{b} = \mathbf{0} \tag{2.2}$$

Where $\boldsymbol{\sigma}$ is the stress tensor and $\mathbf{b}$ is the vector of body forces.

Internal energy balance for the medium

The equation for internal energy balance for the porous medium is established taking into account the internal energy in each phase (E_s, E_l, E_g):

$$\frac{\partial}{\partial t}\left(E_s \rho_s (1-\phi) + E_l \rho_l S_l \phi + E_g \rho_g S_g \phi\right) + \nabla \cdot (\mathbf{i}_c + \mathbf{j}_{Es} + \mathbf{j}_{El} + \mathbf{j}_{Eg}) = f^Q \tag{2.3}$$

Where, $\mathbf{i}_c$ is energy flux due to conduction through the porous medium, the other fluxes ($\mathbf{j}_{Es}$, $\mathbf{j}_{El}$, $\mathbf{j}_{Eg}$) are advective fluxes of energy caused by mass motions and f^Q is an internal/external energy supply.

3.2 Constitutive equations and equilibrium restrictions

In addition to the above given equations, there is a set of necessary constitutive and equilibrium laws. *Table 3.1* summarizes the constitutive laws and the equilibrium restrictions that have to be incorporated. The dependent variables that are computed using each of the laws are also included in this table. The constitutive equations establish the link between the independent variables (or unknowns) and the dependent variables.

Table 3.1: Constitutive equations and equilibrium restrictions.

EQUATION	VARIABLE NAME	VARIABLE
Constitutive equations		
Darcy's law	liquid and gas advective flux	q_l, q_g
Fick's law	vapour and air non-advective fluxes	i_g^w, i_l^a
Fourier's law	conductive heat flux	i_c
Retention curve	liquid phase degree of saturation	S_l, S_g
TEP model	Stress tensor	$\boldsymbol{\sigma}$
Phase density	liquid density	ρ_l
Gases law	gas density	ρ_g
Equilibrium restrictions		
Henry's law	Air dissolved mass fraction	ω_l^h

4 MATERIAL PARAMETERS FOR SAND-BENTONITE MIXTURE

In Agus [1], samples made of 50% sand and 50% bentonite are used to determine the parameters for the Barcelona Basic Model, [2]. The bentonite is Calcigel whose mineralogy composition is similar to the bentonite used by Manju [7] in her tests. That is why we use the TEP model parameters from Agus [1] for the sensitivity analysis and as first guess in the back analysis. Hydraulic parameters are obtained by regression analysis of the Arifin's test results, [4]. Thermal conductivity is taken as from FEBEX, [12].

4.1 Mechanical parameters

Thermoelastoplastic (TEP) model parameters for unsaturated soils are presented in *Table 4.1* and *Table 4.2*.

Table 4.1: TEP Elastic Parameters

κ_{io} [(b)]	κ_{so}	ν	α_{ss} [(b)]	α_i [(b)]	α_{sp} [(b)]	α_o [(T)]
-	-	-	-	-	-	$^oC^{-1}$
0.0029	0.1426	0.3	-0.1128	-0.006	-0.3	1.10^{-5}

Table 4.2: TEP Plastic Parameters

$\lambda(0)$	r	β	ρ [(T)]	k	p^c	M	α	p_o^* [(b)]
-	-	MPa-1	$^oC^{-1}$	-	MPa	-	-	MPa
0.083	0.5165	1.372	0.2	7.32E-03	3.39	1.412	0.426	4.139

[(b)] : This parameter will be used for back analysis.
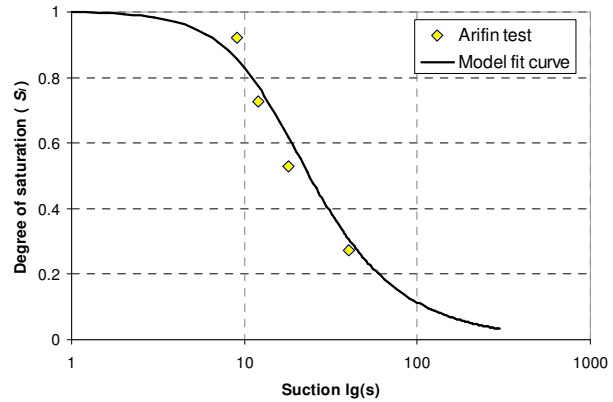[(T)] : This parameter is only used in THM analysis.

4.2 Thermal parameters

The basic parameter for temperature evolution and distribution is the thermal conductivity λ, which depends on liquid saturation S_l [*Fig. 4.1*]. Following [12] we use, $\lambda_{sat} = 1.507 (WmK^{-1})$ and $\lambda_{sat} = 1.0 (WmK^{-1})$.
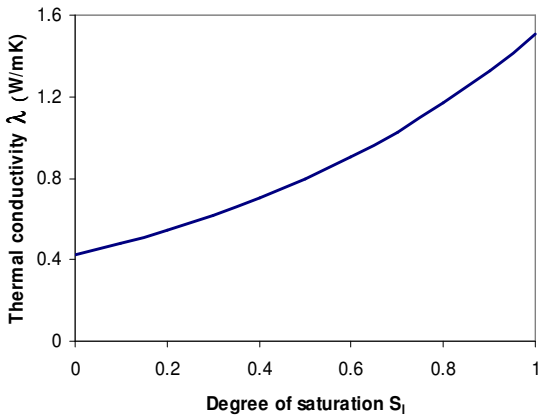
$$\lambda = \lambda_{sat}^{S_l} . \lambda_{dry}^{(1-S_l)}$$

Fig.4.1: Thermal conductivity

$$S_e = \frac{S_l - 0}{1 - 0} = \left(1 + \left(\frac{s}{P_o}\right)^{\frac{1}{1-\lambda}}\right)^{-\lambda}$$

Fig. 4.2 : Retention curve

4.3 Hydraulic parameters

Retention curve

Soil water characteristic curve is obtained based on the results of experiments reported in [4]. The water retention curve is expressed via the well known two parameters of Van Genuchten model, [15]. The parameters obtained via regression analysis and are shown in *Table 4.3*.

Intrinsic permeability:

Intrinsic permeability is calculated by Kozeny's model. Parameters for this model are presented in *fig. 4.3*. Where, k_o is initial intrinsic permeability.

Liquid phase relative permeability

Relative permeability of sand-bentonite mixture is determined in Van Genuchten model as *Fig. 4.4*. Where S_e is the effective degree of saturation, ϕ is porosity, and $\lambda = 0.53$.

$$\mathbf{k} = k_o \frac{\phi^3}{(1-\phi)^2} \frac{(1-\phi_0)^2}{\phi_0^{\,3}}$$

$$k_{rl} = \sqrt{S_e}\left(1-\left(1-S_e^{1/\lambda}\right)^{\lambda}\right)^2$$
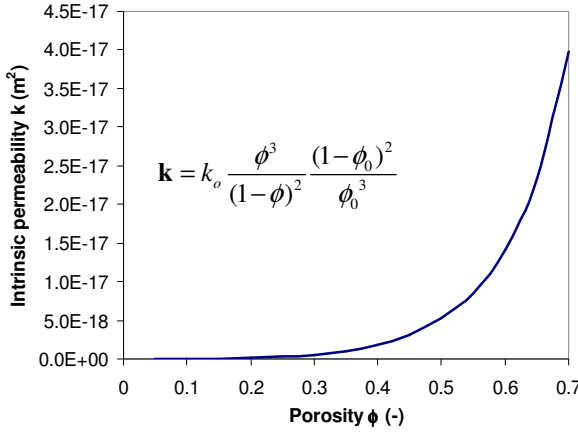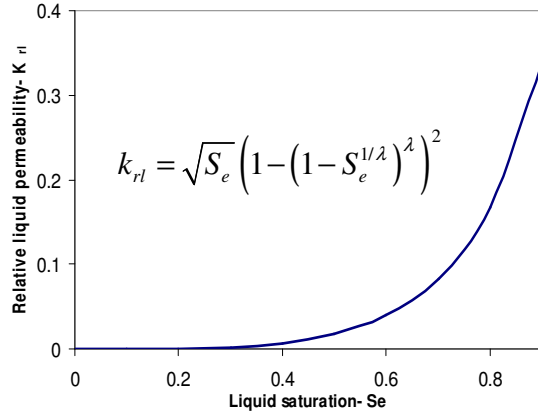
Fig. 4.3: Intrinsic permeability model   Fig 4.4: Relative permeability model

Molecular diffusion of vapour

The molecular diffusion of vapour in air is governed by the Fick's law. The diffusion coefficient is with dimension (m^2/s);

$$D_m^{vapor} = D\tau \left(\frac{(273.15+T)^n}{P_g} \right) \qquad (m^2/s) \tag{4.1}$$

where, D and n are parameters; τ is coefficient tortuosity; Pg is gas pressure (Pa) and T is temperature (^{o}C).

Table 4.3: Hydraulic parameters:

$P_o^{(b)}$	$\lambda^{(b)}$	$k_o^{(b)}$	$D^{(b)(T)}$	$\tau^{(b)(T)}$	$n^{(b)(T)}$	ϕ_0
MPa	-	(m^2)	($m^2 s^{-1} K^{-n} Pa$)	-	-	-
15	0.53	2.07×10^{-19}	$5.9 * 10^{-6}$	0.8	2.3	0.228

(b) : This parameter will be used for back analysis.
(T) : This parameter is only used in THM analysis.

Phase properties parameters are presented in *Table 4.4*, *4.5*.

Table 4.4: Solid phase properties:

$C_s^{(T)}$	874	J kg^{-1} K^{-1}	Solid phase specific heat
ρ_s	2700	kg m^{-3}	Solid phase density
$\alpha_s^{(T)}$	1.20E-05	^{o}C^{-1}	Linear thermal expansion coefficient for grains
$T_o^{(T)}$	20	^{o}C	Reference temperature for thermal expansion

Table 4.5: Liquid phase properties:

ρ_{lo}	1000	kg m^{-3}	Reference density
β	4.5 10^{-4}	MPa^{-1}	Compressibility
$\alpha^{(T)}$	-3.4 10^{-4}	^{o}C^{-1}	Volumetric thermal expansion coefficient for water
γ	0.6923		Solute variation
P_{lo}	0.1	MPa	Reference pressure

$^{(T)}$: This parameter is only used in THM analysis.

5 NUMERICAL SIMULATION

5.1 Simulation of HM test

Numerical modeling

The model is built in the X-Y plane [*fig 5.1*]. The problem is solved as axisymmetric with an axis of symmetry along AD, Y axis-symmetry. At the top and the bottom of the model flux boundary condition is applied, therefore, the discretization there is finer. The distances from points 1, 2, 3 to the top of the model are 50mm, 150mm, 250mm respectively. Points 1, 2 and 3 correspond to the position of the water content and temperature sensors in the sample [See *fig. 2.1 and 5.2(a)*]. Discretization is done in such way to have at the beginning of the simulation the coordinates of the measurement points to coincide with FE-node coordinates. Point 4 is located on the bottom of the sample and it is chosen to collect data corresponding to the load cell measurements.

Boundary conditions are as follows: no displacements in Y-direction on boundary lines AB and CD, corresponding to the bottom and top of the

Fig. 5.1: Model identification

specimen respectively. No displacements in X-direction on boundary line BC and symmetry condition at AD. Water pressure of $P_l = 10$ kPa is applied on line CD corresponding to the top of the specimen. The primary unknowns are displacement vector (U) and liquid pressure (P_l).
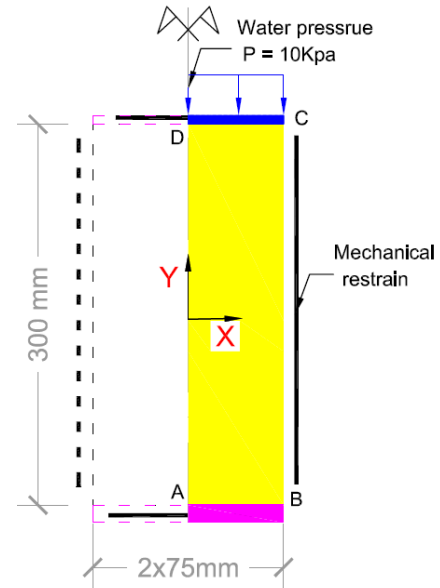
Table 5.2: Initial condition

	Initial void ratio	Initial suction	Temperature (constant)
Unit	-	MPa	^{o}C
Value	0.4077	21.51	20

Simulation result before optimization

    Fig. 5.3 presents the comparison between the calculated and measured degree of saturation. In the experiment, the vertical stress is measured by means of the load cell at the top and the bottom of the soil sample. Therefore, the calculated vertical stress S_{yy} is recorded at point 4 (P4) to be compared with the measurement result in the experimental data [*fig. 5.4*]. The model parameters of the numerical simulation are taken from other papers [1] [4] [12], and this may be the reason for the difference between measurement and simulation stress curves. The agreement between measured and calculated results may be improved by means of back analysis and optimization procedure as it is shown in section 6.2.
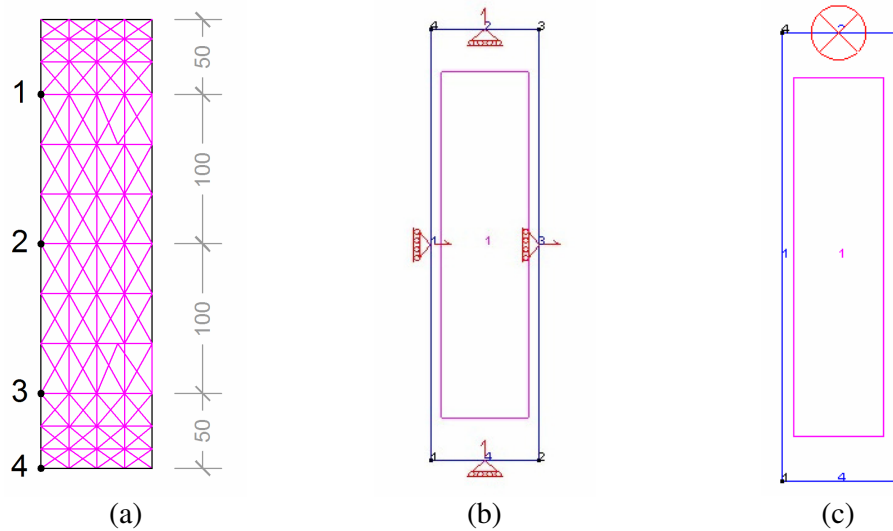

(a)   (b)   (c)

Fig. 5.2: (a) Discretization (points (P) 1,2,3, and 4) are point analysis; (b) Mechanical boundary conditions; (c) Flux boundary conditions.
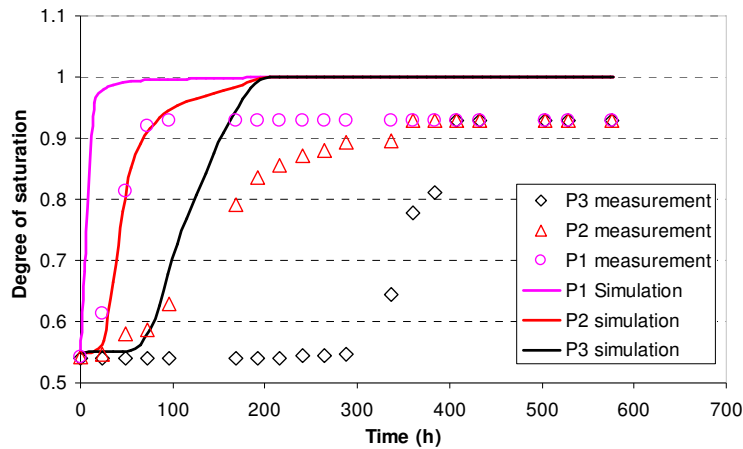

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Fig. 5.3: Evolution of degree of saturation: measurements vs. simulations
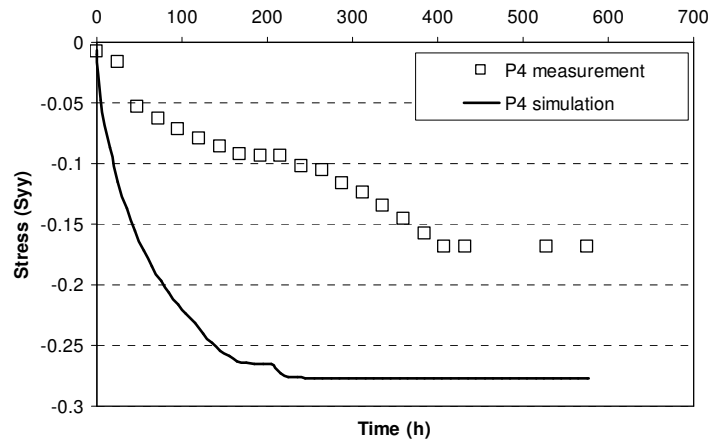

Fig. 5.4: Evolution of vertical stress: measurements vs. simulations

5.2 Simulation of THM test

Numerical modeling

The model geometry is similar as the geometry in previous section. Boundary conditions and initial conditions are presented in *Table 5.3* and *Table 5.4*.

Table 5.3: Boundary conditions

Boundary	Mechanical	Flux boundary
AB	U_y restraint	Constant T = 80°C
BC	U_x restraint	Zero fluxes
CD	U_y restraint	Constant T = 25°C
DA	U_x restraint	Zero fluxes

Table 5.4: Initial conditions

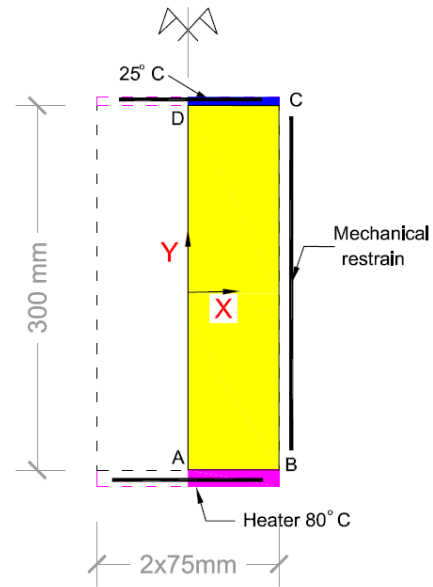| Parameters	Unit	Value
Initial void ratio	-	0.3963
Initial suction	MPa	18.0
Temperature	°C	25
Initial volumetric stress	MPa	-0.15

Fig. 5.5: Model identification

The independent variables are displacement vector (U), liquid pressure (P_l) and temperature (T). Gravity is taken into consideration.

THM simulation results

Measured and computed values of temperature and degree of saturation in the selected points are compared. Points 1, 2 and 3 is placed at 250, 150, and 50 mm respectively from the heater, thus temperature has different values in these points. *Fig. 5.6* presents the evolution of temperature calculated using the model parameter set before applying back analysis of the experimental data. *Fig. 5.7* depicts the evolution of degree of saturation at different points for the same set of not optimized parameter set. When the soil sample is heated by the heater, water in the lower part of the sample (point 3) is evaporated and the

vapor moves in direction to the upper part of the sample. Therefore, the lower part has a trend to dry and the upper part becomes wetter. There is a difference between the numerical simulations and the measured results. This difference may be due to not correct set of parameters used in the simulation.
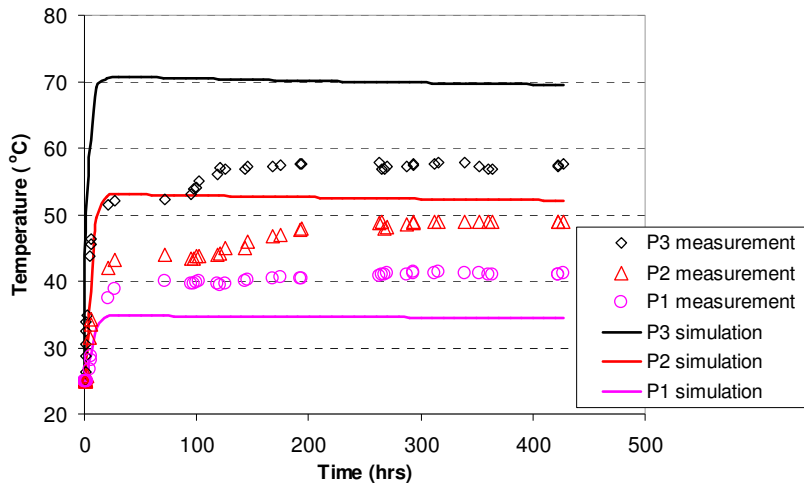

Fig. 5.6 Temperature evolution: simulation vs. measurement (point ith (Pi))
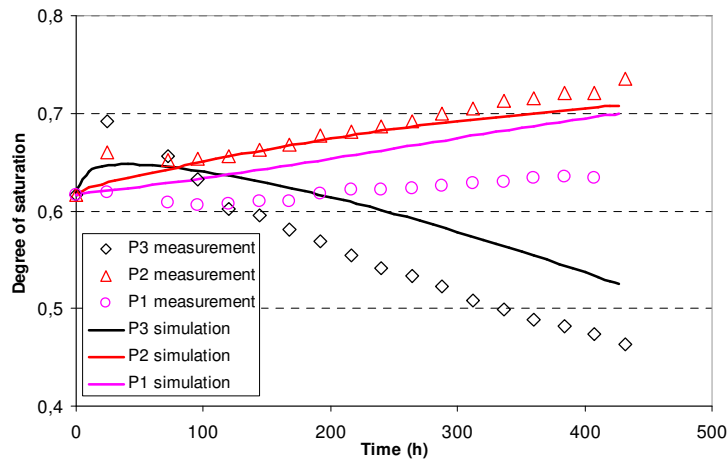

Fig. 5.7: Degree of saturation evolution: simulations vs. measurements

6   SENSITIVITY ANALYSIS AND BACK ANALYSIS

6.2   Sensitivity analysis

Aim of the sensitivity analysis is to estimate the rate of changes in the output of a given model with respect to changes in the model input. Such knowledge is important for evaluating the applicability of the model and for understanding the behaviour of the system being modeled. Sensitivity analysis applied to a prescribed set of boundary and initial conditions problems provides information for the model parameters that need specific measurements, precision and amount of data. Base on the sensitivity analysis the set of the parameters is selected for identification via back analysis. More details and literature review may be found in [14] and [16].

The steps for sensitivity analysis are as follows:

1- Determination of scaled sensitivity (SS): The *SS* analysis indicates the amount of information provided by the *i-th* observation for the estimation of *j-th* parameter. The scaled sensitivity $SS_{i,j}$ of the y_i observation to the model parameter x_j is defined by:

$$SS_{i,j} = \left(\frac{\partial y_i}{\partial x_j}\right) \cdot x_j \sqrt{w_i} \tag{6.1}$$

Weighting factor ω_i is related to the *i-th* observation and is evaluated based on some statistics, i.e. variance, standard deviation or coefficient of variation of the error of the observations.

2- Determination of composite scaled sensitivity (CSS): While the scaled sensitivity (*SS*) refers to one local observed point of interest, the composite scaled sensitivity (*CSS*) gives the sensitivity by root mean square of all observed points:

$$CSS_j = \sqrt{\frac{1}{N}\sum_{i=1}^{N} SS_{i,j}^2} \tag{6.2}$$

3- Determination of factor γ_j for each of parameters: For comparing *CSS* values the following measure is used:

$$\gamma_j = \frac{CSS_j}{max(CSS)} \tag{6.3}$$

Sensitivity analysis for sand-bentonite mixture model

The THM simulation is selected to do the sensitivity analysis. Points (A, B, C, D, E) are selected for this analysis [*Fig. 5.7*]. For the sensitivity analysis, the parameters are catergorized to three groups as follows:

Group 1: parameters influencing liquid flow:

Initial suction *(s_{ini})*, initial porosity (ϕ_{ini}),initial intrinsic permeability *(k)*, vapour diffusion parameter(*D*), thermal boundary condition, liquid boundary condition, λ in retention curve, P_0 in retention curve, λ for relative permeability *(9 parameters)*

Points B, C, D, E are selected for this analysis.

Group 2: parameters influencing thermal conductivity:

Initial suction *(s_{ini})*, thermal boundary condition, initial porosity (ϕ_{ini}), initial intrinsic permeability *(k_o)*, thermal conductivities λ_{dry} and λ_{sat}, and vapour diffusion parameter(*D*), *(7 parameters)*. Point B, C, D are selected.
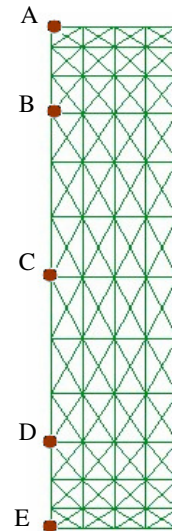

Fig. 6.1: Points analysis

Group 3: parameters influencing the vertical stress S_{yy}:

Initial suction (s_{ini}), thermal boundary condition, initial porosity (ϕ_{ini}), initial intrinsic permeability (k_o), vapour diffusion parameter (D), initial elastic slope for specific volume-mean stress (κ_{io}), initial elastic slope for specific volume-suction (κ_{so}), the parameter for κ_s-(α_{ss}) and (α_{sp}), the parameter for κ_i - (α_i), the parameter for elastic thermal strain (α_o), thermal conductivities λ_{dry} and λ_{sat}, liquid boundary condition. *(14 parameters)*

Points A, B, C, D and E are selected for this analysis.

Ten percent variation is chosen for disturbing the initial parameter set, that is:

$$P_{new} = P_{initial} + 10\% P_{initial} \qquad (6.4)$$

where, P_{new} is the varied parameter; $P_{initial}$ is the initial reference value of the parameters.

Time interval for numerical sensitivity analysis is 427 hours corresponding to the time intervals in Manju's test, [7] .

Results

The summary of the results are given in *Fig. 6.1*, *Fig. 6.2* and *Fig. 6.3* present graphically the values of the factor γ_j for each of the chosen parameters.

The parameter influencing the most the evolution of degree of saturation is the initial porosity [*Fig. 6.1*]. Therefore it is the porosity that mainly controls the water transferring process. Temperature evolution is the most sensitive to thermal boundary condition and secondly to vapour diffusion parameter (D), [*Fig. 6.2*]. Stress distribution is influenced the most by temperature boundary condition. Beside that, α_{ss}, vapour diffusion parameter(D), initial intrinsic permeability (k_o) and initial suction (s_{ini}) also play important roles in the stress evolution [*Fig.6.4*].
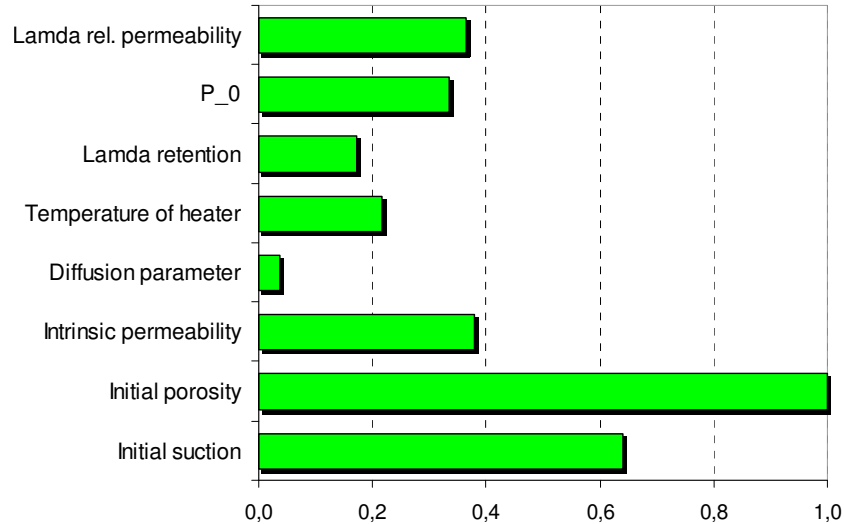

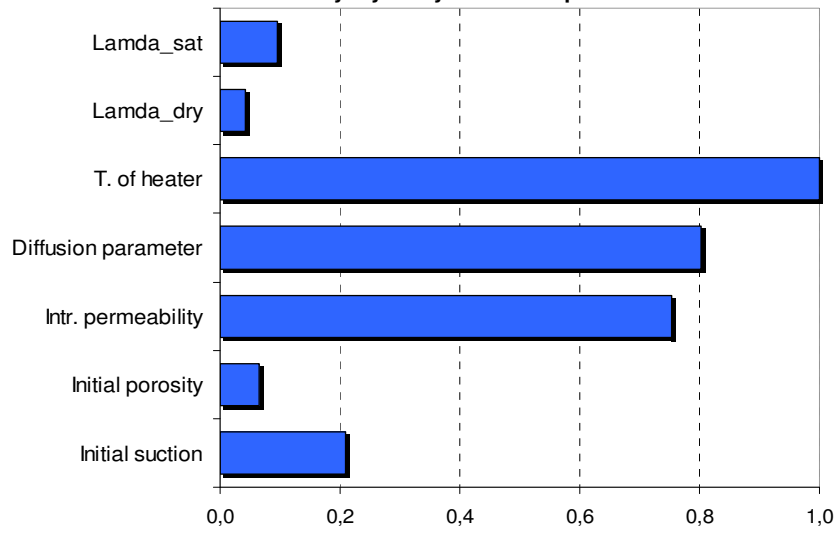Fig. 6.2: γ values for the evolution of degree of saturation with respect to the parameters in group 1

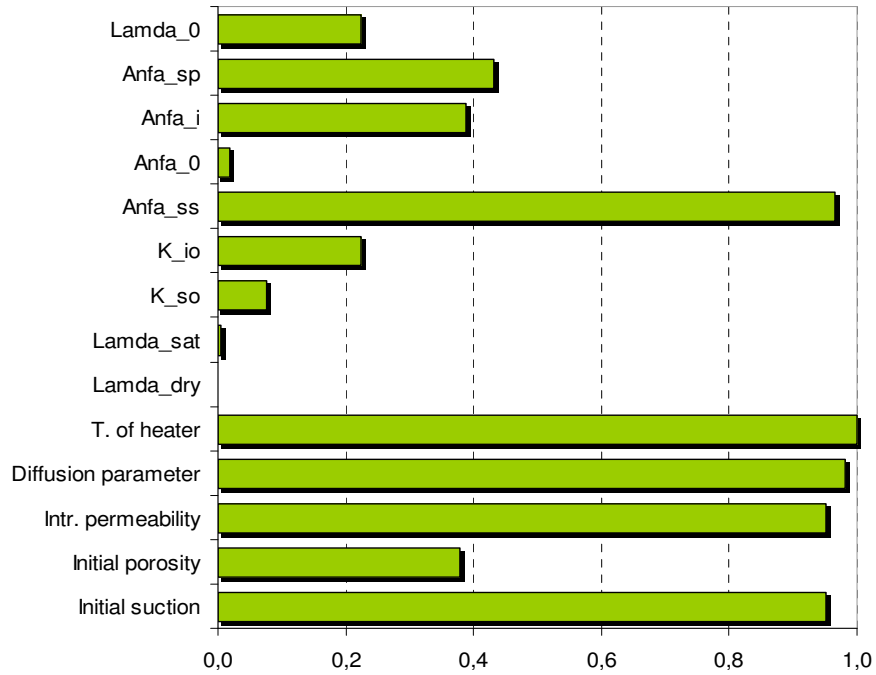Fig. 6.3: γ values for the temperature evolution with respect to the parameters in group 2

Fig. 6.4: γ values for the vertical stress evolution with respect to the parameters in group 3

6.2 Back analysis

For the back analysis approach, a direct approach, which consists of an iterative procedure correcting the trial values of the unknown parameters by minimizing error functions, is applied. The unknown parameters are found when the error function satisfies the impose criteria. The algorithm to solve the optimization problem used here is Neldel-Mead simplex method and we used the optimization routines from the Varocon optimization tool [9].

6.2.1 Back analysis for the HM model:

Selection of parameters

This section presents the optimization or back analysis of HM model presented in the section 5. The measured and reported by Manju [7] degree of saturation and vertical stress are chosen for the back analysis. The model responses and the experimental data are shown in *Fig. 5.3* and *Fig. 5.4*. Totally there are 4 sets of data used for the analysis.

It has been discussed in section 5.1 that based on the performed sensitivity analysis, the evolution of degree of saturation and the vertical stress S_{yy} depend to a greater extend on the following parameters: initial liquid pressure (P_l), initial porosity (ϕ_{ini}), initial intrinsic permeability (k_o), vapour diffusion parameter(D), thermal boundary condition, liquid boundary condition, λ in retention curve, P_0 in retention curve, λ relative permeability, initial elastic slope for specific volume-mean stress curve (κ_{io}), initial elastic slope for specific volume-suction (κ_{so}), parameter for κ_s - (α_{ss}) and (α_{sp}), parameter for κ_i - (α_i), parameter for elastic thermal strain (α_o), thermal conductivities λ_{dry} and λ_{sat}. Initial preconsolidation mean stress (p_0^*) is taken into account, because it also effect on swelling process.

The parameters in retention curve (λ, P_0) have already been determined by fitting curve of Arifin's test, [4]. Initial porosity, in fact, is incorporated in the definition of the intrinsic permeability [Fig. 4.2]. The temperature is supposed to be constant during this simulation and it is taken as reported in the experiment: T = 20 ^{o}C.

Therefore the chosen parameters for further optimization are k_{0i}, α_{ss}, α_i, α_{sp}, κ_{io}, p_0^*. Time interval for back analysis is selected about 576 hours corresponding to the experiment period. Maximum degree of saturation is set to 0.928 corresponding to Manju's measurement [7].

Results and discussion

The back calculated parameters as well as the initial guess for the optimization procedure are given in *Table 6.1*. The best fit to the experimental data for the degree of saturation and vertical stress is shown in *Fig. 6.5* and *Fig. 6.6*. It can be seen that the agreement between measured and calculated S_l is acceptable in P1 and P2. The evolution of the degree of saturation in point 3 (P3) does not match the experimental data within the time interval from 150 to 360 hours. There is a good agreement between the measured and calculated vertical stress at point P4.

Table 6.1: Input and output parameters of the optimization

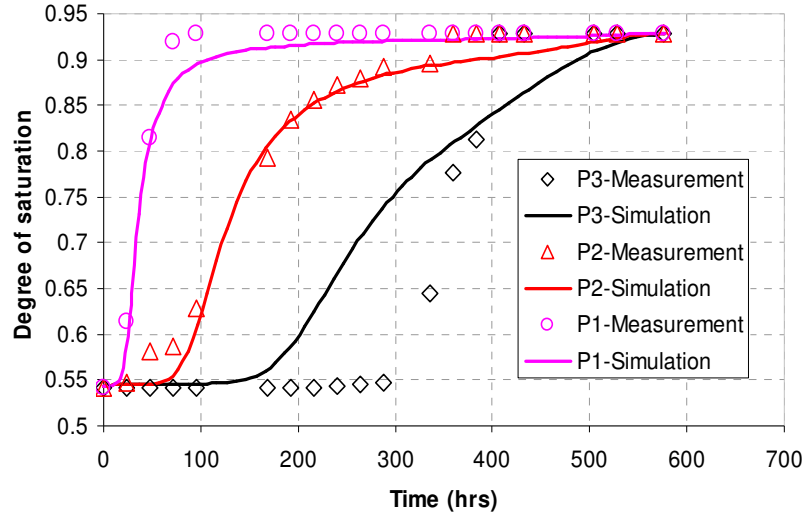| Parameter	Initial	Final	Parameter	Initial	Final
k_{22} (m^2)	2.07E-19	2.65E-20	α_i	-0.006	-0.0067
k_{11}, k_{33} (m^2)	2.07E-19	2.52E-19	α_{sp}	-0.3	-3.40E-01
α_{ss}	-0.1128	-0.1151	κ_{io}	0.0029	3.11E-03
			p_0^* (MPa)	4.139	4.40E+00

Fig. 6.5: the evolution of degree of saturation: simulations vs. measurements
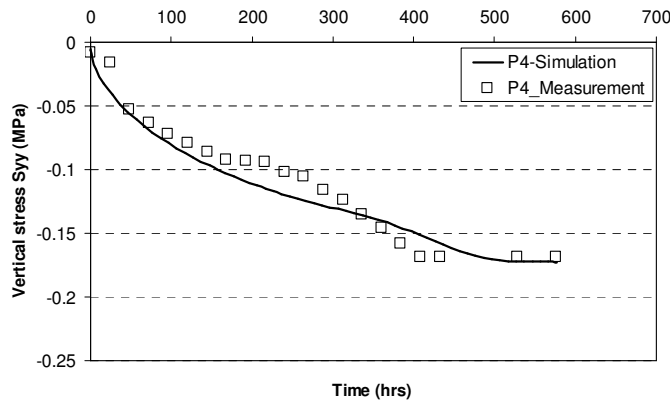

Fig. 6.6:The evolution of vertical stress: simulations vs. measurements

6.2.2 Back analysis for THM model

The parameters used for the back analysis in the THM coupled model are listed in *Table 6.2* and they are chosen based on the sensitivity analysis reported in the section 6.2. Regarding the performed earlier sensitivity analysis of THM model, the parameters are chosen as follows: Diffusion coefficients (*D, n*, and τ); it is assumed that the intrinsic permeability k_o is isotropic and $k_o=k_{11}=k_{22}=k_{33}$; and λ_{sat}, λ_{dry}. The numerical model presented in section 5.2 is used for the back analysis. Time interval for back analysis is selected about 427 hours corresponding to the experiment period.

Fig. 6.7 shows a good agreement between the measured and calculated with the optimized model parameters temperature distribution. However, the calculated degree of saturation is not matching the measured data well especially in P1 but the overall saturation process is described satisfactorily. [*Fig. 6.8*].

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Table 6.2: Input and output parameters of the optimization

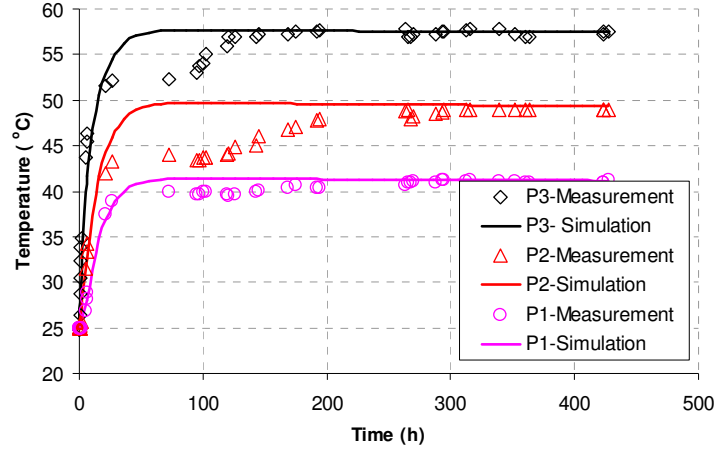| Parameter	Initial	Final	Parameter	Initial	Final
k_o (m^2)	2.07E-19	2.65E-20	D (m^{2}s^{-1}K^{-n}Pa)	5.9E-6	6.44E-05
λ_{sat} (WmK^{-1})	1.5	1.69	τ (-)	0.8	0.911
λ_{dry} (WmK^{-1})	1	1.21	n (-)	2.3	2.8

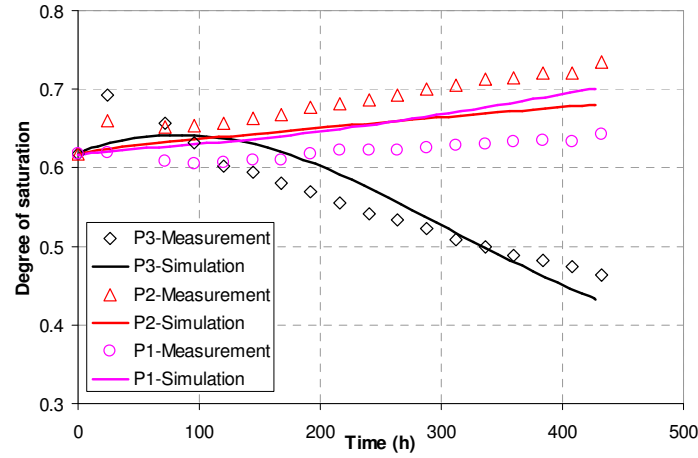Fig. 6.7: The evolution of temperature: simulations vs. measurements

Fig. 6.8: The evolution of degree of saturation: simulations vs. measurements

6.2.3 Final parameters of sand-bentonite mixture model.

From HM and THM back analysis, two sets of parameters are obtained. One parameter might have the different values in different back analysis results, but the model parameters for sand-bentonite mixture are unique. Statistics are proposed to use if there are more than three value of a parameters obtained. The mean value of parameters is calculated in other cases. The two sets of parameters achieved by back analysis have one common parameter that is initial intrinsic permeability (k_o). The mean value is calculated to obtain the unique initial intrinsic permeability value for sand-bentonite mixture. The new set of parameters for sand- bentonite mixture is shown on *Table 6.3, 6.4*. The other parameters, which are not mentioned in these tables, are the same with the initial parameters, [*section 4*].

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Table 6.3: Final thermal and hydraulic parameters

Parameters	k_o	λ_{sat}	λ_{dry}	D	n	τ
Unit	m^2	WmK^{-1}	WmK^{-1}	$m^2 s^{-1} K^{-n} Pa$	-	-
Value	2.65E-20	1.69	1.21	6.44E-05	2.3	0.911

Table 6.4: Final mechanical parameters

Parameters	α_{ss}	α_i	α_{sp}	κ_{io}	p_0^*
Unit	-	-	-	-	MPa
Value	-0.1151	-0.0067	-0.340	3.11E-03	4.40

7   CONCLUSIONS

In this paper, numerical simulations of coupled THM unsaturated soil problems involving barrier materials for nuclear waste repositories have been carried out. Two laboratory tests on HM and THM behavior of sand-bentonite mixture are used for model validation, calibration and verification.

Sensitivity analysis is performed in order to investigate the responses of the models under the variation of some initial conditions, boundary conditions and constitutive model parameters. Sensitivity analysis of THM coupled model shows that the parameter influencing the most the degree of saturation evolution is the initial porosity. Thus, porosity controls mainly the water transfer process. It has been found that the evolution of temperature is the most sensitive to the variation of thermal boundary condition and secondly to the vapour diffusion parameter (D). The stress distribution is influenced mostly by the temperature boundary conditions. Beside that, α_{ss} in TEP model, vapour diffusion parameter (D), initial intrinsic permeability (k_o) and initial suction (s_{ini}) also play important role in the evolution of the vertical stress.

We apply direct back analysis to identify the model parameters to which the model response is the most sensitive. For improvement of the results and for assessing the goodness of the model fit, this method requires more experimental data from HM and THM experiments. Further statistics has to be applied to assess the uniqueness of the obtained optimal sets of parameters.

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