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Persistent URL: http://dml.cz/dmlcz/703070

MATHEMATICAL MODELING OF HYGRO-THERMAL PROCESSES IN DEFORMED POROUS MEDIA

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Abstract: In this contribution we propose a model of coupled heat and moisture transport in variable saturated deformed porous media. Solution of this model provides temperature, moisture content and strain as a function of space and time. We present the detailed description of the model and a numerical illustrative example.

Keywords: hygro-thermo-mechanical model, porous media, initial-boundary problem

MSC: 76S05, 80M10, 80A20

1. Introduction

Phenomena involving coupled transport processes in deformed porous media are important in civil and transport engineering as well as agriculture and ecology. In the past a considerable effort has been invested into developing a fully generalised model describing these phenomena. For related models including thermal creep and chemical deterioration of porous media at high temperatures and fire see e.g. [3] and [5]. In this contribution we extend our work [1] and we propose a coupled model describing moisture and heat transport in partially saturated deformed concrete. The presented model is based on mass and energy conservation law and it is completed by appropriate equilibrium equations. In order to describe the interplay between damage and the transport processes and the material elasticity degradation, respectively, we adopt a straightforward damage model, using mechanical damage parameter as well as thermal damage parameter.

2. Mathematical model

Let Ω be a bounded domain in $\mathbb{R}^2$ with Lipschitz boundary Γ. Let Γ_3 and Γ_4 be open disjoint subsets of Γ. Let $\vartheta \in (0, \infty)$ be fixed throughout the text, $I = (0, \vartheta)$ and $\Omega_\vartheta = \Omega \times I$ denotes the space-time cylinder, $\Gamma_\vartheta = \Gamma \times I$, $\Gamma_{3\vartheta} = \Gamma_3 \times I$ and

$\Gamma_{4\vartheta} = \Gamma_4 \times I$. Let us also mention that throughout the text we use the standard Einstein summation convention. The mathematical model consists of the following equations

$$\frac{\partial \theta(h)}{\partial t} = \nabla \cdot (K(h, T, \boldsymbol{u}) \nabla h) \qquad \text{in } \Omega_\vartheta, \qquad (1)$$

$$c(h, T)\frac{\partial T}{\partial t} = \nabla \cdot (\lambda(h) \nabla T) + c_\ell \, K(h, T, \boldsymbol{u}) \nabla h \cdot \nabla T \qquad \text{in } \Omega_\vartheta, \qquad (2)$$

$$\frac{\partial \sigma_{ij}(h, T, \boldsymbol{u})}{\partial x_j} + b_i = 0, \quad i = 1, 2, \qquad \text{in } \Omega_\vartheta. \qquad (3)$$

Equation (1) represents the moisture balance law, equation (2) represents the energy balance law and equation (3) is the equilibrium equation. In (1)–(3) θ [-] is the moisture retention, h [m] is the pressure head, K [m s $^{-1}$] the hydraulic conductivity, T [°C] denotes the temperature, $\boldsymbol{u} = [u_1; u_2]$ [m] is the vector of displacements, c [J m^{-3}K^{-1}] the volumetric heat capacity of the sample, λ [W m^{-1}K^{-1}] the thermal conductivity, c_ℓ [J m^{-3}K^{-1}] the volumetric heat capacity of water, $\boldsymbol{\sigma} = \sigma_{ij}$ [Pa] is the symmetric elastic stress tensor and $\boldsymbol{b} = [b_1; b_2]$ [N m^{-3}] is the volume force. The model is completed by the appropriate boundary conditions

$$-K(h, T, \boldsymbol{u}) \nabla h \cdot \boldsymbol{n} = \alpha_h(h - h_\infty) \qquad \qquad \text{in } \Gamma_\vartheta, \qquad (4)$$

$$-\lambda(h) \nabla T \cdot \boldsymbol{n} = \alpha_T(T - T_\infty) \qquad \qquad \text{in } \Gamma_\vartheta, \qquad (5)$$

$$-\sigma_{ij} n_j = t_i, \qquad \qquad i = 1, 2, \qquad \text{in } \Gamma_{3\vartheta}, \qquad (6)$$

$$u_i = \bar{u}_i, \qquad \qquad i = 1, 2, \qquad \text{in } \Gamma_{4\vartheta}, \qquad (7)$$

and initial conditions

$$h = h_0 \qquad \text{in } \Omega, \qquad (8)$$

$$T = T_0 \qquad \text{in } \Omega, \qquad (9)$$

$$\boldsymbol{u} = \boldsymbol{u}_0 \qquad \text{in } \Omega. \qquad (10)$$

In (4)–(7) $\boldsymbol{n} = [n_1; n_2]$ denotes the outward unit normal vector, α_h [s^{-1}] is the coefficient of moisture transfer, h_∞ [m] is the ambient matric potential, α_T [W m^{-2}K] the heat transfer coefficient, $\boldsymbol{t} = [t_1; t_2]$ [N m^{-1}] is the surface forces vector and $\bar{\boldsymbol{u}} = [\bar{u}_1; \bar{u}_2]$ [m] is the vector of prescribed displacement. In (8)–(10) h_0 [m] is the initial pressure head, T_0 [°C] is the initial temperature and $\boldsymbol{u}_0 = [u_{01}; u_{02}]$ [m] is the initial displacement.

3. Constitutive relations

In this section we will describe the constitutional relationships for moisture retention, moisture and thermal fluxes and mechanical behavior of the model.
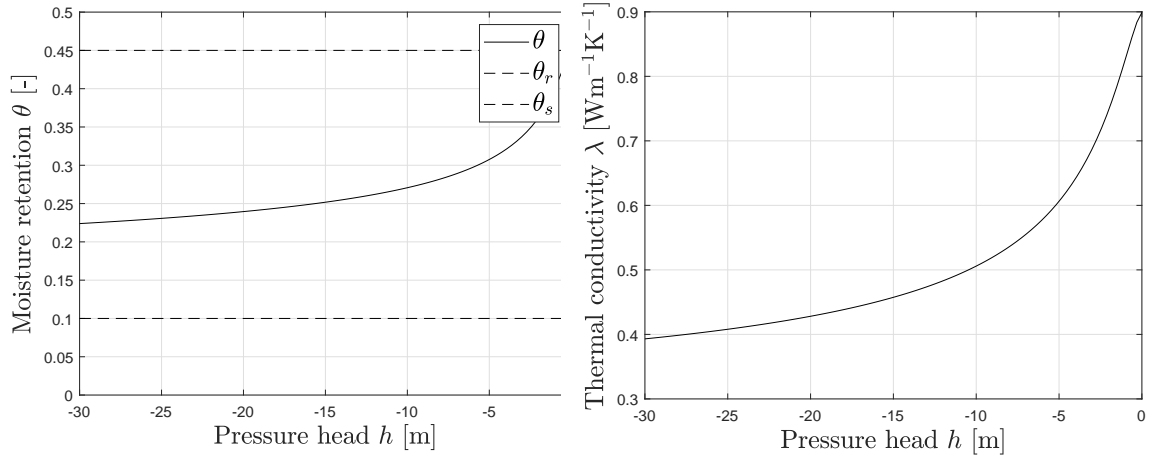
Figure 1: The moisture retention (left) and the thermal conductivity (right) dependance on the pressure head

3.1. Heat and moisture transport behavior

The moisture retention (see Figure 1) is given by van Genuchten relation [6] $\theta(h) = \theta_r + (\theta_s - \theta_r)(1 + |\xi h|^n)^{-m}$, where θ_r [-] is the residual retention, θ_s [-] the saturated retention and ξ [m^{-1}], m [-], n [-] are the empirical parameters of the van Genuchten relation. This relation is applicable for the partially saturated porous media, e.g. zones with negative pressure head. The thermal conductivity (see Figure 1) is given by [4]

$$\lambda(h) = C_1 + C_2\theta(h) - (C_1 - C_4)\exp(-(C_3\theta(h))^{C_5}), \tag{11}$$

where C_1, C_2, C_4 [Wm^{-1}K^{-1}] and C_3, C_5 [-] are the empirical parameters. The hydraulic conductivity is given by [2]

$$K(h, T, \boldsymbol{u}) = K_0(h)10^{4(1-D(T,\boldsymbol{u}))}, \tag{12}$$

where K_0 [ms^{-1}] is the initial permeability and D [-] the multiplicative thermo-mechanical damage parameter. The initial permeability is given by [4] $K_0(h) = k_s\sqrt{S_e(h)}\left(1 - \left[(1 - S_e(h)^{1/m})^m\right]^2\right)$, where k_s [ms^{-1}] is the saturated hydraulic conductivity and $S_e(h) = (1 + |\xi h|^n)^{-m}$. The thermo mechanical damage parameter is defined as $D(T, \boldsymbol{u}) = \omega(T, \boldsymbol{u}) + \chi(T) - \omega(T, \boldsymbol{u})\chi(T)$, where ω [-] is the mechanical damage parameter defined in (15) and χ [-] is the thermal damage parameter defined in (16). The evaluation of the damage parameters is further discussed in the Section 3.2.

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3.2. Mechanical strains and damage parameters

In order to analyze the interplay between the damage and the transport phenomena we introduce a simple damage model taking into account the reduction of the elastic stiffness. The elastic stress tensor is defined as

$$\sigma_{ij} = [1 - \omega(T, \boldsymbol{u})][(1 - \chi(T)]E_{ijkl}\epsilon_{kl}^e, \tag{13}$$

$$\epsilon_{ij}^e = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \delta_{ij}\alpha_\epsilon(T - T_0), \tag{14}$$

where E_{ijkl} [Pa] is the symmetric tensor of initial elastic moduli, ϵ_{ij}^e [-] is the elastic strain tensor. In order to evaluate the damage parameters ω [-] and χ [-] we follow [5]. The mechanical damage function ω is defined as

$$\omega(T, \boldsymbol{u}) = 1 - \frac{\kappa_0}{\kappa(T, \boldsymbol{u})}\exp\left[-\gamma(\kappa(T, \boldsymbol{u}) - \kappa_0)\right], \tag{15}$$

where γ [-] is the fracture release rate, its values for concrete varies around value 100. Further in (15) κ [-] is the damage history parameter taking the maximum value attained by the modified equivalent von Mises strain $\tilde{\epsilon}(T, \boldsymbol{u})$ (for details see [5, p. 722]) or threshold κ_0 [-] which is defined as the ratio between the tensile strength and the Young's modulus (for details see [5, p. 723]). It follows from [5, pp. 723, 728] that dealing with temperatures lower than 50°C we may neglect the temperature dependance of the threshold κ_0 and the fracture release rate γ.

The thermal damage parameter χ [-] is defined as [2, equation (30)]

$$\chi(T) = \zeta_1(T - T_0) - \zeta_2(T - T_0)^2, \tag{16}$$

where $\zeta_1 = 2 \times 10^{-3}$ K^{-1} and $\zeta_2 = 10^{-6}$ K^{-2}.

4. The approximate solution

In order to solve the problem (1)-(10) we formulate the variational form of the stationary problem. Let $0 = \psi^0 < \psi^1 < \cdots < \psi^M = \vartheta$ be an equidistant partitioning of the time interval $[0; \vartheta]$ with time step τ. We set a fixed integer n such that $1 \leq n \leq M$. We denote $f(\boldsymbol{x}, \psi^n)$ by f^n. The time discretization is accomplished through the semi-implicit scheme. Successively for $n = 1, \ldots, M$, for given $[h^{n-1}, T^{n-1}] \in L^\infty(\Omega) \cap W^{1,2}(\Omega)$ and $[u_1^{n-1}, u_2^{n-1}] \in [\bar{u}_1^{n-1}; \bar{u}_2^{n-1}] + W_D^{1,2}(\Omega)$ we search $[h^n, T^n] \in L^\infty(\Omega) \cap W^{1,2}(\Omega)$ and $[u_1^n, u_2^n] \in [\bar{u}_1^n; \bar{u}_2^n] + W_D^{1,2}(\Omega)$, where by $W_D^{1,2}(\Omega)$ we denote the space $W^{1,2}(\Omega)$ of functions with zero trace on Γ_4, such that

$$\int_\Omega \frac{\theta(h^n) - \theta(h^{n-1})}{\tau}\phi_1 \,\mathrm{d}x + \int_\Omega K(h^{n-1}, T^{n-1}, \boldsymbol{u}^{n-1})\nabla h^n \cdot \nabla\phi_1 \,\mathrm{d}x$$
$$+ \int_\Gamma \alpha_h(h^n - h_\infty^n)\phi_1 \,\mathrm{d}x = 0, \quad (17)$$

$$\int_\Omega c(h^{n-1}, T^{n-1})\frac{T^n - T^{n-1}}{\tau}\phi_2\,\mathrm{d}x + \int_\Omega \lambda(h^{n-1})\nabla T^n \cdot \nabla\phi_2\,\mathrm{d}x + \int_\Gamma \alpha_T(T^n - T^n_\infty)\phi_2\,\mathrm{d}x$$

$$- \int_\Omega c_\ell K(h^{n-1}, T^{n-1}, \boldsymbol{u}^{n-1})\nabla h^{n-1} \cdot \nabla T^{n-1}\phi_2\,\mathrm{d}x = 0, \quad (18)$$

$$\int_\Omega \sigma^n_{1i}\frac{\partial\phi_3}{\partial x_i}\,\mathrm{d}x + \int_\Omega b^n_1\phi_3\,\mathrm{d}x + \int_{\Gamma_3} t^n_1\phi_3\,\mathrm{d}x = 0, \quad (19)$$

$$\int_\Omega \sigma^n_{2i}\frac{\partial\phi_4}{\partial x_i}\,\mathrm{d}x + \int_\Omega b^n_2\phi_4\,\mathrm{d}x + \int_{\Gamma_3} t^n_2\phi_4\,\mathrm{d}x = 0, \quad (20)$$

holds for any $[\phi_1, \phi_2, \phi_3, \phi_4] \in W^{1,2}(\Omega)$.

5. Numerical solution

The semi-implicit time discretization leads to the system of nonlinear equations

$$\frac{1}{\tau}C^{n-1}\left(X^n - X^{n-1}\right) + K^{n-1}X^n + R\left(X^n\right) = F^n, \quad (21)$$

where $X^n = (h^n, T^n, u^n_1, u^n_2)$ is the vector of unknown nodal values of matric potential, temperature and displacements in time ψ_n. The constant matrices C^{n-1}, K^{n-1}, F^n and the nonlinear term $R\left(X^n\right)$ consist of the element integral contributions related to the local approximation. This system of equations is solved using the Newton method in each time step. Let us denote

$$\Phi(X^n) = \left[C^{n-1} + \tau K^{n-1}\right]X^n - \tau R\left(X^n\right) - C^{n-1}X^{n-1} - \tau F^n.$$

The solution in the $(k+1)$-th iteration is

$$X^n_{(k+1)} = X^n_{(k)} - J^\Phi_{-1}(X^n_{(k)})\Phi(X^n_{(k)}), \quad (22)$$

where J^Φ denotes the Jacobian matrix of Φ, containing partial derivatives "$J^\Phi = \nabla_X\Phi(X^n)$".

6. Numerical example

In this section we present a numerical example illustrating the applicability of the presented model. For simplicity we assume the plane stress problem with a square domain Ω representing the concrete retaining wall fixed at the bottom, holding the mass of wet soil at the right side. The domain is exposed to an ambient temperature, moisture retention (through an ambient matric potential, e.g. the wet fully saturated soil) and surface forces, see Figure 2. In the Table 1 there are physical parameters.

The spacial discretization of the domain is carried out by means of the FE method with triangular elements with piecewise linear approximation. The numerical procedure has been implemented in Matlab. The time step is set $\tau = 240\,\mathrm{s}$. In Figure 3 we can see the displacement u_1 and the displacement u_2 after 12 hours. In Figure 4

$$\alpha_h = 10^{-20} \text{ s}^{-1}, h_\infty = -1 \text{ m}$$
$$\alpha_T = 10 \text{ Wm}^{-2}\text{K}^{-1}, T_\infty = 50°\text{C}$$
$$t_2 = -200 \text{ kN m}^{-1}$$

$$\alpha_h = 10^{-20} \text{ s}^{-1}$$
$$h_\infty = -1 \text{ m}$$
$$\alpha_T = 10 \text{ Wm}^{-2}\text{K}^{-1}$$
$$T_\infty = 50°\text{C}$$

$$h_0 = \text{-15m}$$
$$T_0 = 10°\text{C}$$

$$\alpha_h = 10 \text{ s}^{-1}$$
$$h_\infty = -1 \text{ m}$$
$$\alpha_T = 10^{-20} \text{ Wm}^{-2}\text{K}^{-1}$$
$$T_\infty = 50°\text{C}$$
$$t_1 = -300 \text{ kN m}^{-1}$$

$$\bar{u}_1 = 0 \text{ mm}$$
$$\bar{u}_2 = 0 \text{ mm}$$
$$\alpha_h = 10^{-20} \text{ s}^{-1}, h_\infty = -1 \text{ m}$$
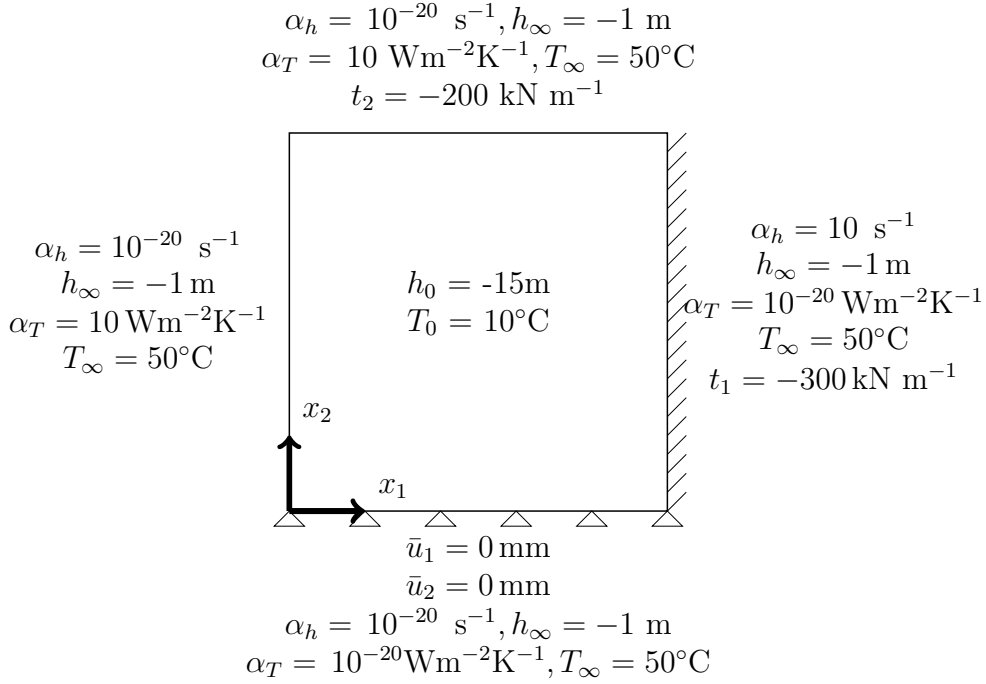$$\alpha_T = 10^{-20} \text{Wm}^{-2}\text{K}^{-1}, T_\infty = 50°\text{C}$$

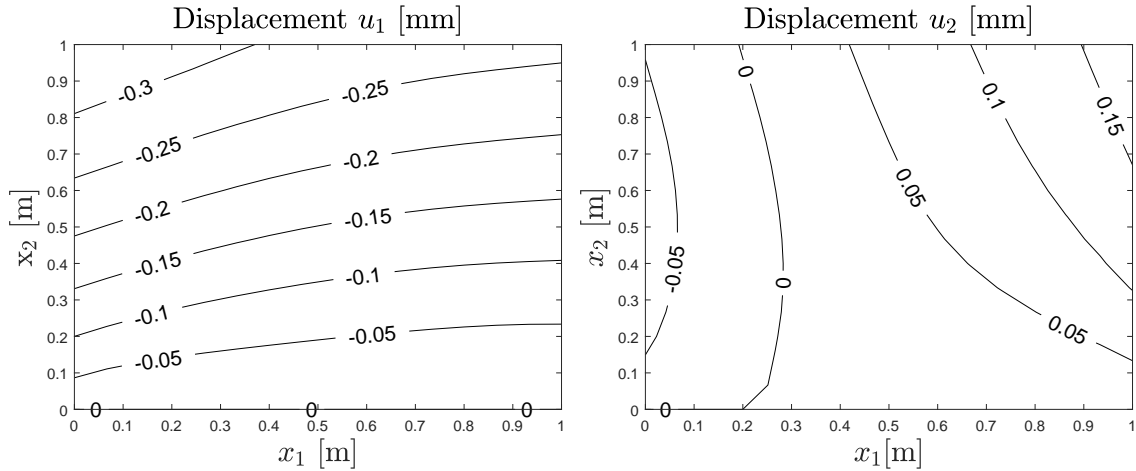Figure 2: The domain Ω, the boundary and initial conditions

Figure 3: The displacement u_1 [mm] (left) and the displacement u_2 [mm] (right)

we can see the moisture retention after 12 hours and the temperature distribution after 2 hours.

The aim of this numerical example was to evaluate the damage influence on the moisture transport processes. The damage is developing mostly due to mechanical loads in the bottom corners of the domain, the temperature contribution to the damage development here is negligible due to relatively low temperature changes during

|	symbol	value	unit
volumetric heat capacity of the sample	c	37.7	$\mathrm{Jm^{-3}K^{-1}}$
volumetric heat capacity of water	c_ℓ	19.9	$\mathrm{Jm^{-3}K^{-1}}$
empirical parameter	C_1	0.55	$\mathrm{Wm^{-1}K^{-1}}$
empirical parameter	C_2	0.8	$\mathrm{Wm^{-1}K^{-1}}$
empirical parameter	C_3	3.07	-
empirical parameter	C_4	0.13	$\mathrm{Wm^{-1}K^{-1}}$
empirical parameter	C_5	4	-
residual moisture retention	θ_r	0.01	-
saturated moisture retention	θ_s	0.11	-
empirical van Genuchten parameter	m	0.2	-
empirical van Genuchten parameter	n	1.48	-
empirical van Genuchten parameter	ξ	1.11	$\mathrm{m^{-1}}$
saturated hydraulic conductivity	k_s	1×10^{-10}	$\mathrm{m\ s^{-1}}$
thermal expansion coefficient	α_ϵ	1×10^{-6}	$\mathrm{K^{-1}}$
fracture release rate	γ	100	-
Young's modulus	E	30	GPa
tensile strength	f_t	3	MPa
compressive strength	f_c	35	MPa
Poisson's ratio	ν	0.2	-

Table 1: Material properties for the illustrative example
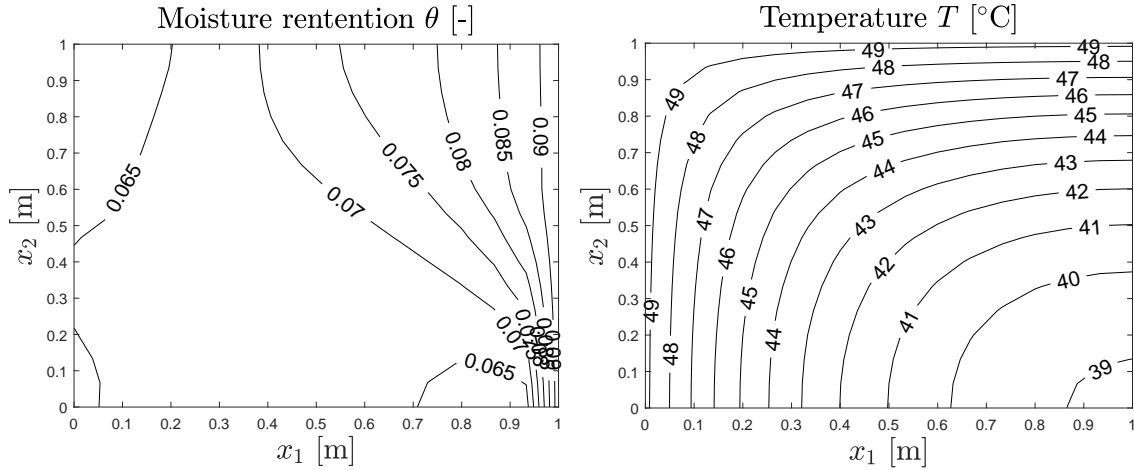
Figure 4: The moisture retention θ [-] (left) and temperature T [°C] (right)

the time of exposure. In Figure 4 we can see the irregularities in the moisture retention field development in the bottom corners caused by this phenomenon. Taking into account the hydraulic conductivity performance we expected the massive mechanical load influence on the transport processes, which has been confirmed by this example.

7. Conclusion

In this contribution we present the coupled thermo-hygro-mechanical model describing coupled transport processes in deformed porous media. The model allows us to evaluate the impact of mechanical and thermal damage on the permeability and mechanical behavior of the medium.

From the moisture retention field we can see the damage influence on the permeability. If we deal with relatively low temperatures the thermal influence on the damage parameter increase (i.e. the permeability decrease) is neglectible. Although imposing the sample to high temperatures (e.g. fire modeling) the thermal influence could prevail over the mechanical one.

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