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NUMERICAL MODELING OF THE SIMULTANEOUS HEAT AND MOISTURE TRANSFER

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Abstract. An original model for the simultaneous transfer of heat and moisture (water in the forms of ice, liquid and vapour) in porous media has been presented in Dalík, Svoboda [1]. In this paper, we briefly describe the model and then present its numerical implementation as well as results of numerical simulation of the process in a brick.

Key words. simultaneous heat and moisture transport in porous media, non–stationary system of non–linear partial differential equations, numerical modeling in a brick

AMS subject classifications. 65M06, 65Z05, 76S05

1. Introduction. The modeling of the process of heat and moisture transfer in porous materials is of essential importance in civil engineering. The most commonly used materials have porous structure and understanding of this process is decisive for the control of durability of building constructions. There exists a lot of reasons why to search after mathematical models enabling simulations of this process under various conditions which can appear in natural and technical systems. The theoretical basis for this modeling has been developed intensively during the last years. Lots of technical papers and in the last years also monographs are devoted to this problem. One of the first and most comprehensive monographs dealing with these processes and their interaction with other processes, especially with soil consolidation, is Lewis, Schrefler [5].

In Section 2, we briefly describe the model and its basic properties. In the following Section 3 we describe the used numerical method and finally, in Section 4, we present results of a numerical simulation.

2. The model. We work with two independent variables $x \in \Omega \subset \mathbb{R}^n, n = 1, 2, 3,$ $t \in (0, t_{\max})$ and as state variables we use the *effective stress*

$$S(x,t) = h(x)g - \frac{\sigma(x,t)}{\varrho(x,t)} \qquad [\mathrm{m}^2\mathrm{s}^{-2}]$$

and *absolute temperature* $T(x,t)$ [K] with

h	[m]	the *height above a chosen fixed level*,
g	$[\mathrm{m\,s^{-2}}]$	the *gravitational constant*,
σ	$[\mathrm{N\,m^{-2}}]$	the *hydrostatic pressure*,
ϱ	$[\mathrm{kg\,m^{-3}}]$	the *density of condensed water*.

The model consists of the following two differential equations

$$\dot{\mathcal{M}} - \nabla(a_{11}\nabla S + a_{12}\nabla T) = 0, \tag{2.1}$$
$$\dot{\mathcal{H}} - \nabla(a_{21}\nabla S + a_{22}\nabla T) = 0, \tag{2.2}$$

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the initial conditions

$$S(x,0) = S_0(x), \qquad T(x,0) = T_0(x), \qquad x \in \Omega \tag{2.3}$$

and the boundary conditions

$$-a_{i1}\frac{\partial S}{\partial \vec{n}} - a_{i2}\frac{\partial T}{\partial \vec{n}} = g^i(x,t,S,T), \qquad x \in \partial\Omega, \qquad t \in (0, t_{\max}), \tag{2.4}$$

which prescribe the intensity of flow of moisture for $i = 1$ and of heat for $i = 2$. The dots over $\mathcal{M}$, $\mathcal{H}$ mean complete time-derivatives, $\vec{n}$ is the outer unit normal vector to the domain Ω,

$$\mathcal{M} = u + \left(\varepsilon - \frac{u}{\varrho}\right)\varphi c_0 \qquad [\mathrm{kg\,m^{-3}}]$$

is the *moisture* in 1 m^3,

u	$[\mathrm{kg\,m^{-3}}]$	is the *amount of condensed water* in 1 m^3
ε	$[-]$	is the *porosity*
φc_0	$[\mathrm{kg\,m^{-3}}]$	is the *amount of vapour* in 1 m^3,

and

$$\mathcal{H} = h_m\varrho_m + h_s u(1-\chi) + h_l u\chi + h_v\left(\varepsilon - \frac{u}{\varrho}\right)\varphi c_0 \qquad [\mathrm{J\,kg^{-3}}]$$

is the *enthalpy* in 1 m^3 with

$$\begin{aligned} h_m = c_m\tau, \quad h_s &= c_s\tau, \quad h_l = L_{sl} + c_l\tau, \\ h_v = L_{sl} + c_l\tau_b &+ L_{lv} + c_v(\tau - \tau_b) \quad [\mathrm{J\,kg^{-1}}]. \end{aligned}$$

The above–used symbols have the following meanings

ϱ_m	$[\mathrm{kg\,m^{-3}}]$	the *mass of the porous material per unit volume*,
c_m	$[\mathrm{J\,kg^{-1}K^{-1}}]$	the *heat capacity of the porous material*,
c_s	$[\mathrm{J\,kg^{-1}K^{-1}}]$	the *heat capacity of the solid*,
c_l	$[\mathrm{J\,kg^{-1}K^{-1}}]$	the *heat capacity of the liquid*,
c_v	$[\mathrm{J\,kg^{-1}K^{-1}}]$	the *heat capacity of the vapour*,
τ_b	$[{}^0\mathrm{C}]$	the *temperature of boiling of water*,
L_{sl}	$[\mathrm{J\,kg^{-1}}]$	the *latent heat of melting* at $\tau = 0\,{}^0\mathrm{C}$ and
L_{lv}	$[\mathrm{J\,kg^{-1}}]$	the *latent heat of evaporation* at $\tau = \tau_b{}^0\mathrm{C}$

and h_m, h_s, h_l, h_v, respectively, means the amount of the enthalpy in 1 kg of porous material, ice, liquid, vapour, respectively. Furthermore,

$$\begin{aligned} a_{11} &= \xi + D & a_{12} &= \frac{D\,L_{lv}}{T} \\ a_{21} &= h_l\xi + h_v D & a_{22} &= \lambda + h_v a_{12} \end{aligned}$$

and ξ, D, λ mean the *conductivity of condensed water, diffusivity of vapour, conductivity of heat*, consecutively. We have found the following formulas for these material characteristics for brick:

$$\begin{aligned} \xi &= 1.23\cdot 10^{-2}\left(\frac{u}{\varrho}\right)^2 \exp\left(-\frac{1883.1}{T}\right) \quad [\mathrm{kg\,m^{-3}s}], \\ D &= 5.05\cdot 10^{-5}T^{-0.19}\left(1 - \frac{u}{\varepsilon\varrho}\right)\exp\left(-\frac{\sigma}{461.9\varrho T} - \frac{5205}{T}\right) \qquad [\mathrm{kg\,m^{-3}s}], \\ \lambda &= 0.45 + (0.185 + 0.0013T)\frac{u}{\varrho} \qquad [\mathrm{J\,m^{-1}s^{-1}K^{-1}}]. \end{aligned}$$

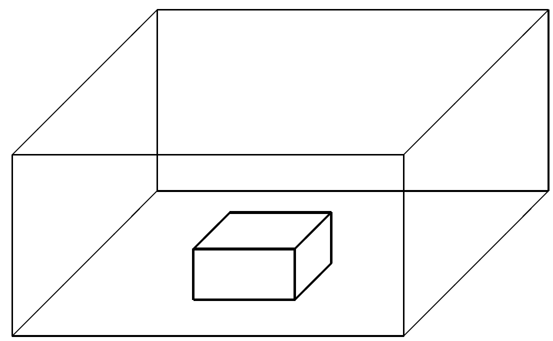

FIG. 2.1. *Schematic experiment.*

As it is apparent from the above descriptions, the properties of the model depend on the function $u = u(S, T)$, called a *sorption isotherme*, essentially. The amount u of condensed water in 1 m^3 of a porous material is a result of an experiment organized as follows. A completely dry specimen of the porous material is included into a space with constant temperature and constant air humidity. See FIG. 2.1. The specimen sucks moisture from the surrounding air and accumulates it in its pores. The end of this process can be identified by the stop of increase of weight of the specimen. It is interesting to note that, if the experiment starts with the specimen filled by water, the final amount of condensed water in its porous structure will be greater than for the dry specimen. This is a consequence of some special microscopic behaviour of the porous structure, as explained in [1]. The sorption isotherme depends on the temperature only weakly, but it is typical that, as a function of σ, it has a hysteresis. A schematic plot of the function u for fixed temperature illustrating these properties can be found in FIG. 2.2. The hysteresis is the smaller, the more homogeneous the porous structure is. These properties of the sorption isothermes are the main reason, why the process of heat and moisture transfer in porous media is strongly non-linear and irreversible.

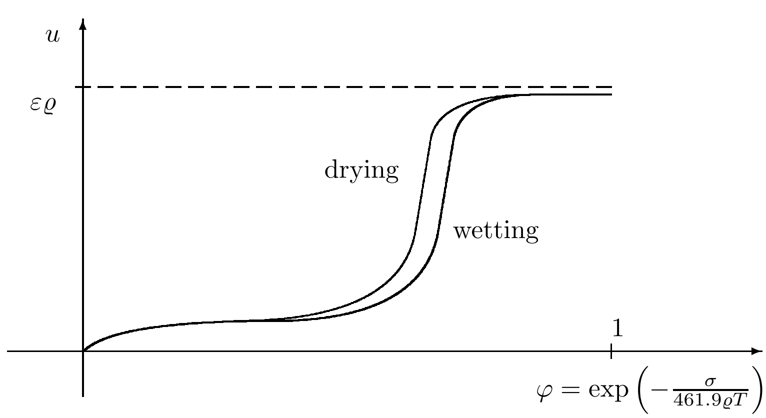

FIG. 2.2. *Typical drying and wetting isothermes for porous materials.*

3. Numerical simulation of the heat and moisture transfer. There exists an extensive amount of various programming systems modeling the process of heat and moisture transport. A systematic development of differential equations for this and similar processes can be found in Lewis, Schrefler [5]. It is applicable to the extension of this model by mechanical deformation of the porous skeleton and by any other related processes. But there exists a theoretical analysis neither of basic properties of the models nor of numerical methods for their approximate solutions. The problem is strongly non-linear and non-potential, so that standard mathematical tools for the existence of exact solution in any sense cannot be used. Certain abstract sufficient conditions for existence of a week solution of problems of this kind have been formulated in Vala [4], but it is not known whether the above problem does really satisfy these conditions. Other technique, used in Dalík, Daněček, Šťastník [2], could possibly give us local existence of the classical solution under rather strong non–realistic smoothness conditions.

In our treatment, we describe a combination of the implicit Euler method for the discretization in time and of the standard finite difference method for the discretization in space. If we put

$$X(x,t) = \begin{pmatrix} S \\ T \end{pmatrix}, \qquad G(x,t,X) = \begin{pmatrix} g_1 \\ g_2 \end{pmatrix}, \qquad O = \begin{pmatrix} 0 \\ 0 \end{pmatrix},$$

$$E(X) = \begin{pmatrix} \dfrac{\partial \mathcal{M}}{\partial S} & \dfrac{\partial \mathcal{M}}{\partial T} \\ \dfrac{\partial \mathcal{H}}{\partial S} & \dfrac{\partial \mathcal{H}}{\partial T} \end{pmatrix} \qquad \text{and} \qquad A(X) = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$$

then we obtain the following forms of the system of equations (2.1), (2.2) and of the boundary conditions (2.4)

$$E(X)\,\dot{X} - \nabla\left(A(X)\,\nabla X\right) = O,$$

$$-A(X)\,\frac{\partial X}{\partial \vec{n}} = G(x,t,X).$$

3.1. Discretization in time. Let us choose a natural number r and put $k = t_{\max}/r$, $t_j = j\,k$ for $j = 0,1,\dots,r$. Instead of $S(x,t)$, $T(x,t)$, we find functions $S^0(x)$, $S^1(x),\dots,S^r(x)$ and $T^0(x)$, $T^1(x),\dots,T^r(x)$ such that the vector-function $X^0(x) = (S^0(x),T^0(x))^\top$ is equal to $(S_0(x),T_0(x))^\top$ and for $j = 1,\dots,r$, the vector-functions $X^j(x) = \left(S^j(x),T^j(x)\right)^\top$ are approximations of the exact solutions $X(x,t_j)$ of the problem (2.1)–(2.4) satisfying the following non-linear boundary–value problem (3.1), (3.2).

$$E(X^j)\,X^j - \nabla\left(kA(X^j)\,\nabla X^j\right) = E(X^j)\,X^{j-1} \quad \text{for} \quad x \in \Omega, \tag{3.1}$$

$$-\,A(X^j)\,\frac{\partial X^j}{\partial \vec{n}} = G(x,t_j,X^j) \quad \text{for} \quad x \in \partial\Omega. \tag{3.2}$$

For a fixed j, we assume that X^{j-1} is known and we solve the problem (3.1), (3.2) by putting $Y_0 = X^{j-1}$ and, consecutively for $i = 1,2,\dots$, by computing Y_i as a solution of the linear boundary-value problem

$$E(Y_{i-1})\,Y_i - \nabla\left(kA(Y_{i-1})\nabla Y_i\right) = E(Y_{i-1})\,Y_0, \tag{3.3}$$

$$-A(Y_{i-1})\frac{\partial Y_i}{\partial \vec{n}} = G(x, t_j, Y_{i-1}) \tag{3.4}$$

and we put $X^j = Y_i$ whenever a certain norm $\|Y_i - Y_{i-1}\|$ is less than a given small positive number.

3.2. Discretization in space. We describe the discretization with respect to the spatial variable x of the problem (3.3), (3.4) for a fixed index i by the standard finite difference method in the case $n = 1$ only. In this case, we denote the interval Ω by (a, b), put $E(x) = E(Y_{i-1})$, $A(x) = A(Y_{i-1})$, $\mathbf{y}(x) = Y_i$, $\mathbf{v}(x) = E(Y_{i-1})\,Y_0$ and $\mathbf{g}(x) = G(x, t_j, Y_{i-1})$, so that the problem (3.3), (3.4) attains the form

$$E(x)\mathbf{y} - k\left(A(x)\mathbf{y}'\right)' = \mathbf{v}(x), \tag{3.5}$$

$$A(a)\mathbf{y}'(a) = \mathbf{g}(a), \qquad -A(b)\mathbf{y}'(b) = \mathbf{g}(b). \tag{3.6}$$

For a natural number m, let $a = x_0 < x_1 < \cdots < x_m = b$ be a uniform mesh with discretization step $h = \frac{b-a}{m}$. By means of the standard finite-difference approximation of the system of equations (3.5), we obtain the linear equations

$$-kA(x_{j-1})\mathbf{y}_{j-1} + \left(2kA(x_j) + E(x_j)h^2\right)\mathbf{y}_j - kA(x_{j+1})\mathbf{y}_{j+1} = h^2\mathbf{v}(x_j) \tag{3.7}$$

for $j = 1, \ldots, m-1$ and discretization of the boundary conditions (3.6) gives us the remaining two equations

$$A(a)(\mathbf{y}_1 - \mathbf{y}_0) = hg(a), \qquad A(b)(\mathbf{y}_{m-1} - \mathbf{y}_m) = hg(b) \tag{3.8}$$

for the unknown approximations $\mathbf{y}_j$ of the vectors $\mathbf{y}(x_j)$ for $j = 0, \ldots, m$.

A possible analysis of discrete solutions of similar non–linear problems is briefly outlined in [5] and the tools presented in the monographs Kurpel [3], Rall [6] may appear to be applicable successfully.

4. Numerical experiment. We are searching for the steady state of the heat and moisture flow in the cross–section of a wall of thickness 0.1 m made from brick with external temperatures $\tau_a(0) = 40\,^0C$, $\tau_a(0.1) = 20\,^0C$, with both surfaces isolated with respect to the flow of moisture and with constant initial temperature $\tau(x) = 30^0C$ and initial relative humidity $\varphi(x) = 0.7$ for $x \in (0, 0.1)$. Hence we use the boundary conditions

$$-\left(a_{11}\frac{\partial S}{\partial x} + a_{12}\frac{\partial T}{\partial x}\right)\vec{n} = 0 \quad \text{and} \quad -\left(a_{21}\frac{\partial S}{\partial x} + a_{22}\frac{\partial T}{\partial x}\right)\vec{n} = \alpha(T - T_a)$$

in the points $x = 0$, $x = 0.1$.

The resulting values of temperature τ and effective stress S in the nodes with even indices appear in TABLE 4.1. Due to our boundary conditions, the sum of flows of liquid and vapour must equal to zero. Our approximations of flows of liquid and vapour in the first and last intervals appear in TABLE 4.2 and schematic illustrations of the graphs of these flows can be found in FIG. 4. These results indicate that the steady state is a dynamic one in the following sense: Vapour flows from places of higher temperature to places of lower temperature (in the positive direction of the x-axis) and then condensates to liquid. The same amount of liquid flows in the opposite direction and then evaporates to vapour. In the following TABLE 4.3, we compare the intensities of heat flow through the porous material skeleton by heat conduction, transported by vapour and by liquid through

i	0	2	4	6	8	10
$\tau(x_i)$	36.506	33.904	31.301	28.699	26.096	23.494
$S(x_i)$	50108.4	50108.3	50108.2	50108.2	50108.1	50108.0

Table 4.1

interval	$[x_0, x_1]$	$[x_9, x_{10}]$
flow of liquid	$-.7973\ 10^{-6}$	$-.3282\ 10^{-6}$
flow of vapour	$.7908\ 10^{-6}$	$.3255\ 10^{-6}$

Table 4.2

medium	porous material	vapour	liquid
heat in [J $m^{-2}s^{-1}$]	75.75	1.35	−0.066

Table 4.3

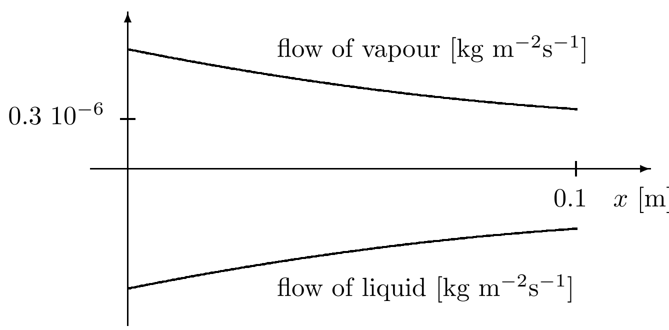

Fig. 4.1. *Steady state of flow of vapour and liquid across the brick wall.*

the middle point x_5. We can see that the heat transported by vapour represents 1.8 % of the heat transported through the porous material skeleton. Of course, this amount may play important role in the thermal bilance of walls made from better insulating porous materials.

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REFERENCES

[1] J. Dalík, and J. Svoboda, *A model for the heat and moisture propagation in porous materials.* Prepared for publication.
[2] J. Dalík, J. Daněček and S. Šťastník, *The Kiessl model, existence of the classical solution. 1.* Matematická štatistika a numerická matematika a ich aplikácie, Zborník konferencie, Kočovce 1999, 62–75.
[3] N. S. Kurpel, *Projection-Iterative Methods for Solution of Operator Equations*, AMS, Providence, RI, 1976.

[4] J. Vala, *On the evolution of heat and moisture in building materials*. Proceedings of Algoritmy (Algorithms), Podbanské, 2002, pp 146–152.

[5] R. W. Lewis and B. A. Schrefler, *The finite element method in static and dynamic deformation and consolidation of porous media*, John Wiley & Sons, Toronto, 1998.

[6] L. B. Rall, *Computational Solution of Nonlinear Operator Equations*, Wiley, New York, 1969.