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ON THE MATHEMATICAL MODELLING OF THE PROCESS OF THE HEAT AND MOISTURE TRANSFER IN THE POROUS MATERIALS

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Математическое моделирование процесса переноса тепла
и влаги в пористых материалах

Предложена конечно-разностная схема для численного решения одной нелинейной математической модели переноса влаги и тепла в пористых материалах. Сформулирована соответствующая начально-краевая задача для стенки из поробетона и определены технические характеристики — количество влаги и ее среднее содержание по времени. Расчеты показывают, что полученные характеристики не зависят от временного и пространственного шагов предложенной разностной схемы. Предложена неявная формула для определения энтальпии h_e таяния льда.

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Pavluš M., Pavlušová E. E11-99-8
On the Mathematical Modelling of the Process of the Heat
and Moisture Transfer in the Porous Materials

The finite difference scheme is suggested for the numerical solution of a non-linear mathematical model which described the simultaneous transfer of the heat and moisture in the porous materials. An appropriate initial-boundary value problem is formulated for a wall of the aired concrete and the technical characteristics like the quantity of the moisture and its mean-time value are determined. The calculations show that the resulted charcteristics do not depend on the time and space steps of the suggested difference scheme. An implicit formula for the determination of the enthaply h_e of the ice melting is suggested.

The investigation has been performed at the Laboratory of Computing Techniques and Automation, JINR.

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1 INTRODUCTION

The most building materials have a part of their volumes filled with small pores connected by narrow channels. This porous structure is able to absorb, save, transport and discharge moisture, which consists of water in the form of ice, liquid and gas. The amount of moisture in the porous structure, which is closely related to temperature, is essential for the durability of materials and stability of building constructions. Hence, there is an extensive need for modelling of the process of moisture and heat transfer in porous materials. Because of this need, several mathematical models of this process have been developed. The first successful attempts appeared in Philip de Vries [1] and Glaser [2] in the late fifties; more historical information can be found in [3] and [4].

In this article we pay attention to the non-linear mathematical model used by Künzel [5] in 1994. We give a short description of the model in Section 2. In Section 3 we formulate needed initial and boundary conditions. We suggest the numerical solution in Section 4 for the created initial-boundary value problem. This numerical solution is based on the finite-difference method. Section 5 describes the technical characteristics like a quantity of the moisture and its mean-time value. We verify numerical results of the problem solution in Section 6 through these technical characteristics if an important civil-engineering material – aired concrete is considered.

2 MATHEMATICAL MODEL

Let us consider the following two differential equations

$$\frac{dw}{d\varphi}\frac{\partial\varphi}{\partial t} = \frac{\partial}{\partial x}\left(D_\varphi\frac{\partial\varphi}{\partial x} + \delta_p\frac{\partial\varphi p_{sat}}{\partial x}\right), \qquad 0 < x < d, t > 0, \tag{1}$$

$$\frac{dH}{d\vartheta}\frac{\partial\vartheta}{\partial t} = \frac{\partial}{\partial x}\left(\lambda\frac{\partial\vartheta}{\partial x}\right) + h_v\frac{\partial}{\partial x}\left(\delta_p\frac{\partial\varphi p_{sat}}{\partial x}\right), \qquad 0 < x < d, t > 0, \tag{2}$$

where φ and ϑ are respectively relative moisture $[-]$, $0 < \varphi < 1$ and temperature $[K]$ given for each point $(x,t) : 0 < x < d$, $t > 0$. φ and ϑ are unknown functions. The notation $[-]$ means a measureless value.

w is a quantity of moisture $[kg/m^3]$ in the given porous material including all phases of the water such that

$$w = w_f\frac{(b-1)\varphi}{b-\varphi}, \tag{3}$$

where w_f is a free saturation by the water in the porous material $[kg/m^3]$, and b is a coefficient of approximation $[-]$, $b > 1$.

D_φ is a coefficient of transport of moisture $[kg/ms]$ given by the formula

$$D_\varphi = D_w\frac{\partial w}{\partial\varphi}, \tag{4}$$

where D_w is a diffusion coefficient $[m^2/s]$.

δ_p is a permeability of water vapour into the porous material $[kg/msPa]$

$$\delta_p = \frac{2.10^{-7}}{\mu p_L}\vartheta^{0.81}, \tag{5}$$

where μ is a water vapour diffusion resistance factor $[-]$, p_L is a pressure of the surroundings $[Pa]$ and p_{sat} is a pressure of the saturated water vapour $[Pa]$

$$p_{sat} = \begin{cases} 611e^{\frac{17.08\vartheta}{234.18+\vartheta}} & \text{if } \vartheta \geq 273.15 \\ 611e^{\frac{22.44\vartheta}{272.44+\vartheta}} & \text{otherwise.} \end{cases} \tag{6}$$

H is an enthalpia $[J/kg]$ of the porous material that is the sum

$$H = H_s + H_w, \tag{7}$$

of the enthalpias for dry and moist material. We suppose that

$$H_s = \varrho_s c_s \vartheta, \tag{8}$$

for the dry material and

$$H_w = \begin{cases} w c_w \vartheta & \text{if } \vartheta \geq 273.15 \\ \vartheta((w - w_e)c_w + w_e c_e - h_e \frac{dw_e}{d\vartheta}) & \text{otherwise,} \end{cases} \tag{9}$$

for the moist material that can contain beside a water, an ice as well. Here c_s, c_w, c_e are respectively heat capacities of dry porous material, of water and of ice $[J/kgK]$, ϱ_s is a density of dry porous material $[kg/m^3]$, h_e is an enthalpia of the ice melting $[J/kg]$, and w_e is a quantity of the ice in the porous material. This quantity can be obtained by substituting from (10)

$$\varphi_e = k.\vartheta + q, \qquad 253.15 < \vartheta < 273.15, \tag{10}$$

to the (3). The relation (10) is received as a result of the experimental data given in [5]. k and q are some constants. Then substituting from w_e to (9), from (9) and (8) to (7) and deriving H with respect to ϑ we have

$$\frac{dH}{d\vartheta} = \begin{cases} \varrho_s c_s + w c_w & \text{if } \vartheta \geq 273.15 \\ \varrho_s c_s + w_f(b-1)\{\frac{c_w}{b-\varphi}[\varphi + \frac{b\vartheta}{b-\varphi}\frac{\partial\varphi}{\partial\vartheta}] & \\ -\frac{c_w - c_e}{b-q-k\vartheta}[q + k\vartheta + \frac{bk\vartheta}{b-q-k\vartheta}] & \\ -\frac{h_e bk}{(b-q-k\vartheta)^2}[1 + \frac{2k\vartheta}{b-q-k\vartheta}]\} & \text{otherwise.} \end{cases} \tag{11}$$

Next,

$$\lambda = \lambda_0(1 + \frac{pw}{\varrho_s}), \tag{12}$$

is a thermal conductivity $[W/mK]$, where λ_0 is a thermal conductivity of dry material, p is a coefficient of the increment of the thermal conductivity $[-]$. Finally h_v is an enthalpia of the water $[J/kg]$.

3 INITIAL AND BOUNDARY CONDITIONS

Let us consider the following initial conditions for unknown functions φ and ϑ

$$\varphi(x,0) = \frac{b_\varphi - a_\varphi}{d}x + a_\varphi, \qquad 0 < x < d, \tag{13}$$

and

$$\vartheta(x,0) = \frac{b_\vartheta - a_\vartheta}{d}x + a_\vartheta, \qquad 0 < x < d, \tag{14}$$

where a_φ, b_φ, a_ϑ, b_ϑ are some real constants and d is a thickness of the material $[m]$. Boundary conditions are as follows

$$\varphi(0,t) = a_\varphi, \qquad t > 0, \tag{15}$$

$$\vartheta(0,t) = a_\vartheta, \qquad t > 0, \tag{16}$$

$$\varphi(d,t) = c_\varphi + d_\varphi sin(\frac{\pi}{2}(\frac{4t}{365} + 1)), \qquad t > 0, \tag{17}$$

$$\vartheta(d,t) = c_\vartheta + d_\vartheta sin(\frac{\pi}{2}(\frac{4t}{365} - 1)), \qquad t > 0, \tag{18}$$

where c_φ, d_φ, c_ϑ, d_ϑ are some real constants.

4 NUMERICAL SOLUTION OF THE PROBLEM

For the domain $(x,t) : 0 < x < d,\ t > 0$ let us consider the following discretization $(x_i, t_n) : x_i = (i-1)h,\ t_n = n\tau$, where $i = 1, 2, \ldots, N, N+1$; $n = 0, 1, \ldots$ and $h > 0$ is a space step of discretization and $\tau > 0$ is a time step of discretization. We denote $\varphi_i^{(n)}$ and $\vartheta_i^{(n)}$ as the approximate values of the exact values $\varphi(x_i, t_n)$ and $\vartheta(x_i, t_n)$. Using common finite-difference approximation for derivatives in equations (1), (2) we obtain two following difference equations

$$\frac{dw}{d\varphi}(\varphi_i^{(n)})\frac{\varphi_i^{(n+1)} - \varphi_i^{(n)}}{\tau} = \frac{1}{h^2}[D_\varphi(\varphi_{i+1/2}^{(n)})(\varphi_{i+1}^{(n+1)} - \varphi_i^{(n+1)}) - D_\varphi(\varphi_{i-1/2}^{(n)})(\varphi_i^{(n+1)} - \varphi_{i-1}^{(n+1)})], \tag{19}$$

$$\frac{dH}{d\vartheta}(\vartheta_i^{(n)}, \varphi_i^{(n+1)})\frac{\vartheta_i^{(n+1)} - \vartheta_i^{(n)}}{\tau} = \frac{1}{h^2}[\lambda(\varphi_{i+1/2}^{(n+1)})(\vartheta_{i+1}^{(n+1)} - \vartheta_i^{(n+1)}) - \lambda(\varphi_{i-1/2}^{(n+1)})(\vartheta_i^{(n+1)} - \vartheta_{i-1}^{(n+1)})], \tag{20}$$

that can be rewritten to the form

$$\varphi_{i-1}^{(n+1)}[\frac{D_\varphi(\varphi_{i-1/2}^{(n)})}{h^2}] - \varphi_i^{(n+1)}[\frac{D_\varphi(\varphi_{i-1/2}^{(n)})}{h^2} + \frac{D_\varphi(\varphi_{i+1/2}^{(n)})}{h^2} + \frac{1}{\tau}\frac{dw}{d\varphi}(\varphi_i^{(n)})] + \varphi_{i+1}^{(n+1)}[\frac{D_\varphi(\varphi_{i+1/2}^{(n)})}{h^2}] = -\frac{\varphi_i^{(n)}}{\tau}\frac{dw}{d\varphi}(\varphi_i^{(n)}), \tag{21}$$

$$\vartheta_{i-1}^{(n+1)}[\frac{\lambda(\varphi_{i-1/2}^{(n+1)})}{h^2}] - \vartheta_i^{(n+1)}[\frac{\lambda(\varphi_{i-1/2}^{(n+1)})}{h^2} + \frac{\lambda(\varphi_{i+1/2}^{(n+1)})}{h^2} + \frac{1}{\tau}\frac{dH}{d\vartheta}(\vartheta_i^{(n)}, \varphi_i^{(n+1)})] + \tag{22}$$

$$+\vartheta_{i+1}^{(n+1)}[\frac{\lambda(\varphi_{i+1/2}^{(n+1)})}{h^2}] = -\frac{\vartheta_i^{(n)}}{\tau}\frac{dH}{d\vartheta}(\vartheta_i^{(n)}, \varphi_i^{(n+1)})],$$

where $i = 2, 3, \ldots, N$; $n = 0, 1, \ldots$ and, for example,

$$D_\varphi(\varphi_{i-1/2}^{(n)}) = [D_\varphi(\varphi_i^{(n)}) + D_\varphi(\varphi_{i-1}^{(n)})]/2,$$

$$\lambda(\varphi_{i+1/2}^{(n+1)}) = [\lambda(\varphi_{i+1}^{(n+1)}) + \lambda(\varphi_i^{(n+1)})]/2.$$

Equations (21), (22) under fixed n lead to the two systems with three-diagonal matrices which can be solved by well known methods of linear algebra.

5 IMPORTANT TECHNICAL CHARACTERISTICS

The quantity of the moisture in the wall of the thickness d at the fixed moment $t \geq 0$ can be determined according to the following formula

$$W(t) = \frac{1}{d}\int_0^d w(x,t)dx \tag{23}$$

where function $w(x,t)$ is expressed by the formula (3). If $t = 0$ then substituting from the initial condition (13) to the (3) we can calculate exact value

$$W(0) = -w_f\frac{(b-1)d}{b_\varphi - a_\varphi}[1 + \frac{b}{b_\varphi - a_\varphi}ln|\frac{b-b_\varphi}{b-a_\varphi}|]. \tag{24}$$

However, if $t > 0$ the integral (23) can be computed only numerically, for example, by the trapezoidal rule

$$W(t) = h[\frac{w(x_1,t)}{2} + w(x_2,t) + w(x_3,t) + \ldots + \frac{w(x_{N+1},t)}{2}] \tag{25}$$

where $w(x_1,t)$ and $w(x_{N+1},t)$ are determined by substituting from boundary conditions (15) and (17) respectively to the (3). The rest of values $w(x_i, t_{n+1})$ $i = 2, 3, \ldots, N$ we determine approximately according to the formula

$$w(x_i, t_{n+1}) = w_f(b-1)\frac{\varphi_i^{(n+1)}}{b-\varphi_i^{(n+1)}}. \tag{26}$$

The final formula is

$$W(t_{n+1}) = w_f(b-1)h[\frac{1}{2}\frac{a_\varphi}{b-a_\varphi} + \sum_{i=2}^{N}\frac{\varphi_i^{(n+1)}}{b-\varphi_i^{(n+1)}} + \frac{1}{2}\frac{c_\varphi + d_\varphi sin(\frac{\pi}{2}(\frac{4t}{365}+1))}{b - c_\varphi - d_\varphi sin(\frac{\pi}{2}(\frac{4t}{365}+1))}]. \tag{27}$$

Other important characteristics is a mean-time value of the quantity of the moisture in the porous material. It can be calculated by the formula

$$\bar{W}(t_{n+1}) = \frac{1}{t_{n+1}}\int_0^{t_{n+1}} W(t)dt. \tag{28}$$

6 CALCULATION RESULTS

We have calculated an example with the following input data for aired concrete: $d = 0.3m$, $b = 1.022$, $w_f = 340kg/m^3$, $D_w = 10^{-8}m^2/s$, $\mu = 8$, $p_L = 10^5Pa$, $\varrho_s = 600kg/m^3$, $c_s = 850J/kgK$, $c_e = 2090J/kgK$, $c_w = 4190J/kgK$, $h_v = 25.10^5J/kgK$, $k = 0.008K^{-1}$, $q = -1.1852$, $\lambda_0 = 0.14W/mK$, $p = 3$. The value h_e can be chosen from the relation

$$\frac{\partial}{\partial\vartheta}[\vartheta(-w_e c_w + w_e c_e - h_e\frac{dw_e}{d\vartheta})] = 0, \qquad \vartheta < 273.15. \tag{29}$$

However, relation (29) provide different values h_e that depend on the fixed point chosen on the line (10). For a fixed point on the line (10) we have just one value of h_e. The correctness of the technical characteristics (27), (28) as well as of the difference scheme (21), (22) we have verified by space and time step changing. The results for the space step h changing are given in the Table 1 if fixed total time is one year ($t = 365$ days, $\tau = 1/24$ day).

h	$d/10$	$d/20$	$d/30$	$d/40$
$\bar{W}(t)$	15.13	15.19	15.21	15.22

Table 1. The dependence of $\bar{W}(t)$ on the space step h

The results for the time step τ changing are given in the Table 2 if the thickness of the material is divided into 30 equal parts ($h = d/30$) and the time unite is one day.

τ	1	1/4	1/12	1/24
$\bar{W}(t)$	15.211	15.206	15.205	15.205

Table 2. The dependence of $\bar{W}(t)$ on the time step τ

Tables 1 and 2 show that the numerical method suggested here for the solution of equations (1) and (2) is stable.
The following figures were drawn for the case of $\tau = 1$ day, $h = d/30$ and a total time of 3×365 days. The figure 1 shows the boundary condition (17) for the relative moisture φ if $c_\varphi = 0.71$, $d_\varphi = 0.13$. The figure 2 shows the boundary condition (18) for the temperature ϑ if $c_\vartheta = 5$, $d_\vartheta = 20$.

Figure 1

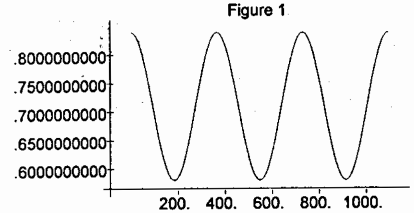


Figure 2

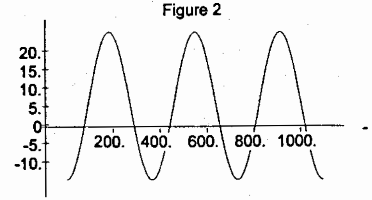


Figure 3

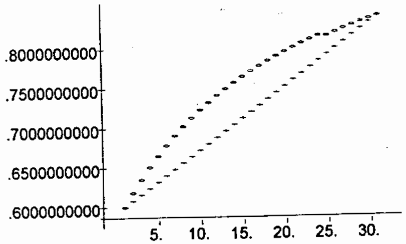
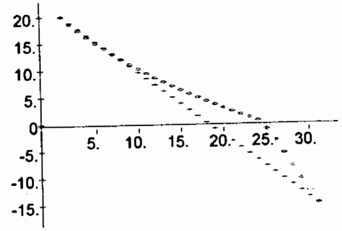


Figure 4



The figure 3 displaies the initial condition (13) for the relative moisture φ denoted by crosses if $a_\varphi = 0.6$, $b_\varphi = 0.84$. The same figure displaies the distribution of the relative moisture φ after three years - ovals. The figure 4 displaies the initial condition (14) for the temperature ϑ if $a_\vartheta = 20$, $b_\vartheta = -15$. The same figure displaies the distribution of the temperature after three years - ovals.

Figure 5

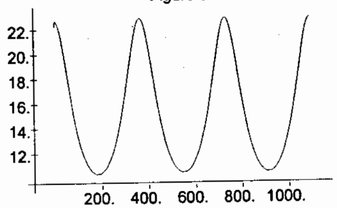
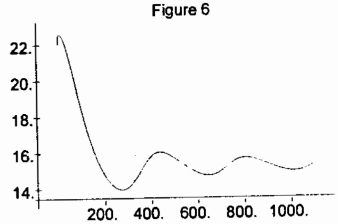


Figure 6



The figure 5 indicates the quantity of moisture in the wall for different time values according to the formula (27). The figure 6 indicates the mean-time value of the quantity of the moisture that was calculated according to the formula (28).

7 CONCLUSION

The calculation results prove that the suggested difference scheme (19) – (20) gives the satisfactory numerical solution of the problem (1) – (2) under the initial and boundary conditions (13) – (14) and (15) – (18) respectively. We verified the formula (29) for choosing the enthalpy h_e not only in the case of aired concrete constants but in the other cases as well. The formula (29) works also satisfactory in these other cases and is a good supplement to the work [5]. The difference scheme, presented in this article, was programmed in Fortran and concerns the modelling total time that is equal to three years (1095 days). The total computational time takes about 12 minutes on the PC with MMX 166MHz processor. We computed also the cases when the modelling total time was five and ten years. The obtained results are similar to the results that we present here.

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