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NUMERICAL IMPLEMENTAION OF A FREEZING-FRONT MODEL FOR WATER-SATURATED MEDIA THAT INCLUDES THE DEPENDENCE OF THE PHASE-TRANSITION TEMPERATURE ON THE PRESSURE AND CONCENTRATION

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A computational algorithm is constructed for solution of the problem of freezing of water-saturated porous media with account for the dependence of the temperature of the phase transition of pore moisture on the pressure and the concentration of a dissolved impurity. The mathematical model of the process considered is based on a generalized formulation of the well-known Stefan problem. Examples convey results of computation.

The behavior of freezing-melting water-saturated media is mainly determined by phase transitions of pore moisture. These transitions are accompanied by migration and diffusion of dissolved impurities. In what follows we consider the dependence of the freezing temperature of the pore moisture on the pressure and the concentration of a dissolved impurity on the interface of the melted and frozen zones. The mathematical model of the process considered is based on a generalized formulation of the well-known Stefan problem [1].

1. The basic relations are the heat-conduction equation for the solid-phase zone

$$\frac{\partial T}{\partial t} = a_s \frac{\partial^2 T}{\partial x^2}, \quad x \in (0, \xi(t)); \tag{1}$$

the equations of heat conduction, piezoconductivity, and diffusion of the impurity dissolved in water for the liquid phase:

$$\frac{\partial T}{\partial t} = a_{liq} \frac{\partial^2 T}{\partial x^2}, \quad x \in (\xi(t), L); \tag{2}$$

$$\frac{\partial p}{\partial t} = \kappa \frac{\partial^2 p}{\partial x^2}, \quad x \in (\xi(t), L); \tag{3}$$

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2}, \quad x \in (\xi(t), L). \tag{4}$$

On the interface $\xi(t)$ of the melted and frozen phases, a moisture discontinuity is considered and the balance of the energy, the mass of water, and the mass of the impurity dissolved in the water is described by the following equations:

$$\lambda_s \left(\frac{\partial T}{\partial x}\right)_- - \lambda_{liq} \left(\frac{\partial T}{\partial x}\right)_+ = q \rho_{ic} m \frac{d\xi}{dt}, \tag{5}$$

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$$\left(\frac{\partial p}{\partial x}\right) = -\left(1 - \frac{\rho_{ic}}{\rho_w}\right)\frac{m}{k_{liq}}\mu\frac{d\xi}{dt}, \tag{6}$$

$$-D\left(\frac{\partial C}{\partial x}\right) = C_*\frac{d\xi}{dt}, \tag{7}$$

$$T = -\alpha C - \eta\,(p - P_a). \tag{8}$$

Let the porous medium considered have a constant temperature, concentration of the dissolved impurity, and pressure in pores at the initial moment:

$$T(x, 0) = T_0, \quad x \in [0, L]; \tag{9}$$

$$C(x, 0) = C_0, \quad x \in [0, L]; \tag{10}$$

$$p(x, 0) = P_a, \quad x \in [0, L]. \tag{11}$$

On the left boundary the water is assumed to cool instantaneously to the constant temperature T_c:

$$T(0, t) = T_c, \quad t > 0,$$

and on the right boundary it is assumed that there are no inflows of heat, concentration of the impurity, and water mass at all:

$$\frac{\partial T}{\partial x} = 0, \quad x = L, \quad t > 0; \tag{12}$$

$$\frac{\partial C}{\partial x} = 0, \quad x = L, \quad t > 0; \tag{13}$$

$$\frac{\partial p}{\partial x} = 0, \quad x = L, \quad t > 0. \tag{14}$$

2. We consider a computational algorithm suitable for effective numerical realization of boundary-value problem (1)-(14) and based on a modified method of counter factorization [2, 3].

On the segment $[0, L]$ the quasiuniform grid $\overline{\omega}_h = \{x_i = x_{i-1} + h_i,\ i = \overline{1, n};\ x_0 = 0;\ h_i = bh_{i-1},\ i = \overline{1, n}\}$ is constructed. Its steps form an increasing geometric progression with the denominator $b > 1$. Here the parameters of the grid n, h_1, and b are chosen so that $x_n = L$. The time step is calculated in the course of solution of the formulated problem.

It is assumed that approximate values of the solution of the initial problem are found up to the time $t = t_{j-1}$. To find the solution of the problem for the time $t = t_j$, we set up a correspondence between Eqs. (1)-(14) and their purely implicit finite-difference analogs

$$\hbar_i\frac{T_i - \overset{\vee}{T}_i}{a_{liq}\tau} = \frac{T_{i+1} - T_i}{h_{i+1}} - \frac{T_i - T_{i-1}}{h_i}, \quad i = \overline{j+1, n-1}; \tag{15}$$

$$\hbar_i\frac{p_i - \overset{\vee}{p}_i}{\kappa\tau} = \frac{p_{i+1} - p_i}{h_{i+1}} - \frac{p_i - p_{i-1}}{h_i}, \quad i = \overline{j+1, n-1}; \tag{16}$$

$$\hbar_i \frac{C_i - \overset{\vee}{C}_i}{D\tau} = \frac{C_{i+1} - C_i}{h_{i+1}} - \frac{C_i - C_{i-1}}{h_i}, \quad i = \overline{j+1, n-1}; \tag{17}$$

$$\hbar_i \frac{T_i - \overset{\vee}{T}_i}{a_s\tau} = \frac{T_{i+1} - T_i}{h_{i+1}} - \frac{T_i - T_{i-1}}{h_i}, \quad i = \overline{1, j-1}. \tag{18}$$

The discrete analog of conjugation condition (8) is written in the form

$$T_j = -\alpha C_j - \eta (p_j - P_a). \tag{19}$$

We set up a correspondence between Stefan condition (5) and its discrete analog, which has the second order of approximation with respect to τ:

$$\lambda_s \frac{T_j - T_{j-1}}{h_j} + \lambda_s \frac{\overset{\vee}{T}_{j-1} - \overset{\vee}{T}_{j-2}}{h_{j-1}} + \lambda_{liq} \frac{T_j - T_{j+1}}{h_{j+1}} + \lambda_{liq} \frac{\overset{\vee}{T}_{j-1} - \overset{\vee}{T}_j}{h_j} = 2mq\rho_{ic} \frac{h_j}{\tau}. \tag{20}$$

Using the recurrence relations

$$\begin{gathered} C_{j+1} = (1 - \alpha^C_{j+1}) C_j + \beta^C_{j+1}, \quad p_{j+1} = (1 - \alpha^p_{j+1}) p_j + \beta^p_{j+1}, \\ T_{j+1} = (1 - \alpha^T_{j+1}) T_j + \beta^T_{j+1}, \quad T_{j-1} = (1 - \alpha^T_j) T_j + \beta^T_j, \end{gathered} \tag{21}$$

the purely implicit finite-difference analog of Eqs. (5)-(7)

$$\lambda_s \frac{T_j - T_{j-1}}{h_j} + \lambda_{liq} \frac{T_{j+1} - T_j}{h_{j+1}} = mq\rho_{ic} \frac{h_j}{\tau}, \tag{22}$$

$$\frac{p_{j+1} - p_j}{h_{j+1}} = -\left(1 - \frac{\rho_{ic}}{\rho_w}\right) \frac{m}{k_{liq}} \mu \frac{h_j}{\tau}, \tag{23}$$

$$-D \frac{C_{j+1} - C_j}{h_{j+1}} = C_j \frac{h_j}{\tau}, \tag{24}$$

and the discrete analog (19), excluding h_j/τ, we obtain a quadratic equation for T_j:

$$\begin{aligned} &\left\{ [1 + \eta\gamma (\lambda_s b\alpha^T_j + \lambda_{liq}\alpha^T_{j+1})] [\lambda_s b\alpha^T_j + \lambda_{liq}\alpha^T_{j+1}] \right\} T_j^2 + \\ &+ \left\{ - [1 + \eta\gamma (\lambda_s b\alpha^T_j + \lambda_{liq}\alpha^T_{j+1})] [\lambda_s b\beta^T_j + \lambda_{liq}\beta^T_{j+1}] + \right. \\ &+ \left[\eta \frac{\beta^p_{j+1}}{\alpha^p_{j+1}} - \eta P_a - \eta\gamma (\lambda_s b\beta^T_j + \lambda_{liq}\beta^T_{j+1}) \right] \left[\lambda_s b\alpha^T_j + \lambda_{liq}\alpha^T_{j+1} \right] - \\ &\left. - mq\rho_{ic} D\alpha^C_{j+1} [1 + \eta\gamma (\lambda_s b\alpha^T_j + \lambda_{liq}\alpha^T_{j+1})] \right\} T_j + \\ &+ \left\{ - \left[\eta \frac{\beta^p_{j+1}}{\alpha^p_{j+1}} - \eta P_a - \eta\gamma (\lambda_s b\beta^T_j + \lambda_{liq}\beta^T_{j+1}) \right] \left[\lambda_s b\beta^T_j + \lambda_{liq}\beta^T_{j+1} \right] + \right. \end{aligned}$$

$$+ mq\rho_{ic}D\alpha^{C}_{j+1}\left[\eta P_a - \eta\frac{\beta^{p}_{j+1}}{\alpha^{p}_{j+1}} + \eta\gamma\lambda_s b\beta^{T}_{j} + \eta\gamma\lambda_{liq}\beta^{T}_{j+1}\right] - mq\rho_{ic}D\alpha\beta^{C}_{j+1}\Bigg\} = 0\,, \tag{25}$$

where

$$\gamma = \frac{(\rho_w - \rho_{ic})\,\mu}{\alpha^{p}_{j+1}\,\rho_{ic}\,\rho_w q k_{liq}}\,.$$

The smaller root of Eq. (25) is taken as the next approximation T_j. Then the unknown p_j and C_j are found correspondingly:

$$p_j = \frac{\beta^{p}_{j+1}}{\alpha^{p}_{j+1}} + \gamma\lambda_s b\,(\alpha^{T}_{j}T_j - \beta^{T}_{j}) + \gamma\lambda_{liq}\,(\alpha^{T}_{j+1}T_j - \beta^{T}_{j+1})\,, \tag{26}$$

$$C_j = -\frac{T_j + \eta\,(p_j - P_a)}{\alpha}\,. \tag{27}$$

The boundary conditions are put in correspondence with their discrete analogs.

For realization of the obtained system at each time level, i.e., at each fixed value of the index j, the iteration process will be organized in view of its nonlinearity. The order of operations is as follows.

Step 1. $k = 0$ (a counter of iterations) is assumed and the initial approximation of the time step τ_0 (usually, $\tau_0 = \tau$) is specified.

Step 2. The simplest linearization of the system of equations (15)-(19) is done:

$$\hbar_i\frac{\overset{k+1}{T_i} - \overset{v}{T_i}}{a_{liq}\tau} = \frac{\overset{k+1}{T_{i+1}} - \overset{k+1}{T_i}}{h_{i+1}} - \frac{\overset{k+1}{T_{i+1}} - \overset{k+1}{T_{i-1}}}{h_i}\,,\quad i = \overline{j+1,\,n-1}\,;$$

$$\hbar_i\frac{\overset{k+1}{p_i} - \overset{v}{p_i}}{\kappa\tau} = \frac{\overset{k+1}{p_{i+1}} - \overset{k+1}{p_i}}{h_{i+1}} - \frac{\overset{k+1}{p_{i+1}} - \overset{k+1}{p_{i-1}}}{h_i}\,,\quad i = \overline{j+1,\,n-1}\,;$$

$$\hbar_i\frac{\overset{k+1}{C_i} - \overset{v}{C_i}}{D\tau} = \frac{\overset{k+1}{C_{i+1}} - \overset{k+1}{C_i}}{h_{i+1}} - \frac{\overset{k+1}{C_{i+1}} - \overset{k+1}{C_{i-1}}}{h_i}\,,\quad i = \overline{j+1,\,n-1}\,;$$

$$\hbar_i\frac{\overset{k+1}{T_i} - \overset{v}{T_i}}{a_s\tau} = \frac{\overset{k+1}{T_{i+1}} - \overset{k+1}{T_i}}{h_{i+1}} - \frac{\overset{k+1}{T_{i+1}} - \overset{k+1}{T_{i-1}}}{h_i}\,,\quad i = \overline{1,\,j-1}\,.$$

For its solution the method of counter factorization is used, in which the solution is sought with the help of the recurrence relations mentioned above:

$$\begin{aligned}
&\overset{k+1}{T_i} = (1 - \alpha^{T}_{i+1})\,\overset{k+1}{T_{i+1}} + \beta^{T}_{i+1}\,,\quad i = \overline{j-1,0}\,;\\
&\overset{k+1}{T_i} = (1 - \alpha^{T}_{i})\,\overset{k+1}{T_{i-1}} + \beta^{T}_{i}\,,\quad i = \overline{j+1,\,n}\,;\\
&\overset{k+1}{p_i} = (1 - \alpha^{p}_{i})\,\overset{k+1}{p_{i-1}} + \beta^{p}_{i}\,,\quad i = \overline{j+1,\,n}\,;
\end{aligned} \tag{28}$$

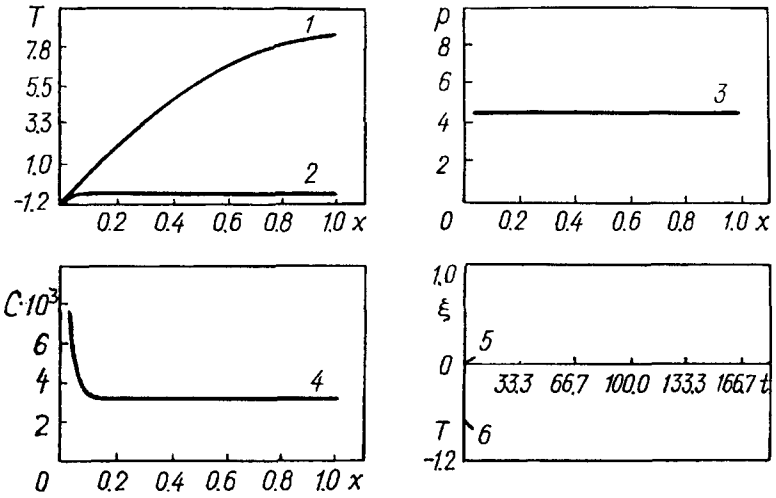

Fig. 1. A case of adequate operation of the model. $T_0 = 10^\circ C$, $T_c = -1^\circ C$, $k_{liq} = 8.5 \cdot 10^{-16}$, $D = 1.45 \cdot 10^{-9}$. x, m; t, days.

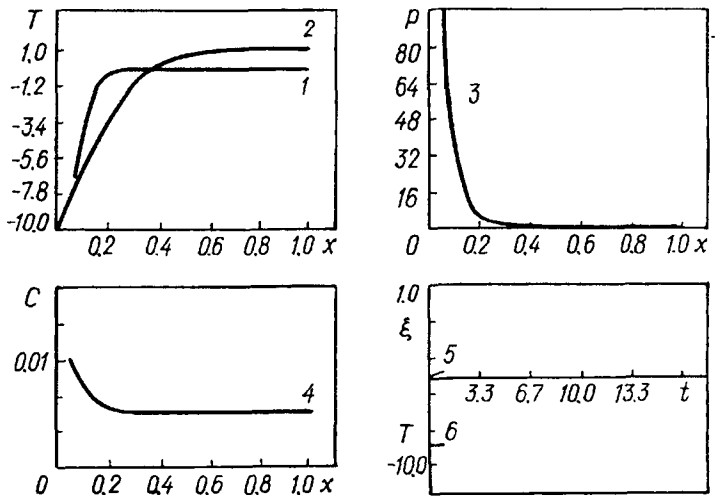

Fig. 2. An example of supercooling. $T_0 = 3^\circ C$, $T_c = -3^\circ C$, $k_{liq} = 8.5 \cdot 10^{-16}$, $D = 1.45 \cdot 10^{-9}$.

$$C_i^{k+1} = (1 - \alpha_i^C)\, C_{i-1}^{k+1} + \beta_i^C, \quad i = \overline{j+1, n}.$$

Step 3. With the use of obtained relations (25)-(27), the next approximation of the temperature, pressure, and concentration of the dissolved impurity on the interface of the melted and frozen phases T_j^{k+1}, P_j^{k+1}, C_j^{k+1} is calculated.

Step 4. The next approximations of the temperature in the frozen zone and the temperature, pressure, and concentration in the melted zone are found from counter-factorization formulas (28).

Step 5. The next approximation of the time step τ^{k+1} is determined from Eq. (20).

Step 6. If the error of the iteration process is

$$\left| \frac{\tau^{k+1}}{\tau^k} - 1 \right| \geq \varepsilon,$$

where ε is a specified small number larger than 0, then k is increased by unity and step 2 is started again. Otherwise, it is assumed that passage to the next time level has occurred.

3. Numerical calculations following the computational algorithm described were carried out for the following parameters of the process studied: $m = 0.2$; $P_a = 10^5$ Pa; $C_0 = 0.003$ g/liter; $\eta = 0.765 \cdot 10^{-7}$; $\alpha = 66.7$; $q = 3.34 \cdot 10^5$; $C_{sk} = 1920$ J/(kg·K); $C_w = 4190$ J/(kg·K); $C_{ic} = 2000$ J/(kg·K); $\rho_w = 1000$ kg/m^3; $\rho_{ic} = 910$ kg/m^3; $\rho_{sk} = 2000$ kg/m^3; $\lambda_w = 0.58$ W/(m·K); $\lambda_{ic} = 2.23$ W/(m·K); $\lambda_{sk} = 2$ W/(m·K); $\mu = 0.001$ Pa·sec; $K_f = 2 \cdot 10^9$ Pa; $L = 1$ m; $h_1 = 10^{-4}$; $k_{liq} = 8.5 \cdot 10^{-15} - 8.5 \cdot 10^{-23}$ m^2; $D = 1.45 \cdot 10^{-9}$ m^2/sec; $\varepsilon = 10^{-5}$.

As can be seen from the graphs (Figs. 1, 2) two different freezing regimes exist. The following notation is used in the figures: 1) temperature, °C; 2) equilibrium temperature, °C; 3) pressure, MPa; 4) concentration, g/liter; 5) interface $\xi(t)$, m; 6) temperature on the interface between the frozen and melted zones, °C. In Fig. 1 one can see results of the computation that show that the present front model describes adequately the occurring process. Figure 2 shows the so called "supercooling" effect. Here, the equilibrium-temperature curve calculated with account for the pressure and concentration distribution lies above the local-temperature distribution curve. In the freezing-front model a supercooling effect is observed for regimes corresponding to strong cooling, when the freezing front moves so rapidly that because of the substantial difference in the diffusion coefficient and the thermal diffusivity and in the piezoconductivity and the thermal diffusivity in the melted zone the salt concentration and the pore pressure decrease more rapidly with distance from the front than the local temperature increases. A comparison with results of [2], where only the temperature and the concentration were calculated, and of [4], where the temperature and the pressure were calculated, shows that the effect of the pressure and the concentration of the impurity in water on the temperature of the phase transition is independnet.

NOTATION

x, coordinate; t, time; T, temperature, C, mass concentration of the impurity in water; p, pressure; m, porosity; μ, viscosity of water; q, specific heat of the phase transition of water; D, diffusion coefficient; ξ, coordinates of the interfaces between the zones; c, heat-capacity coefficient; ρ, density coefficient; λ, thermal conductivity; κ, piezoconductivity; κ_{liq}, permeability of the melted ground; K_f, modulus of compressibility of water; α, η, coefficients of decrease of the phase-transition temperature; h_i, steps of the space grid; $\overline{\omega}_h$, space grid; n, number of nodes of the space grid; L, length of the calculated area; τ, step of the time grid; j, number of the node at which the phase transition occurs; α_i^T, β_i^T, α_i^C, β_i^C, α_i^p, β_i^p, factorization coefficients; k, iteration number; P_a, atmospheric pressure; T_c, boundary condition for the temperature at $x = 0$; $c\rho_s = (1 - m)c_{sk}\rho_{sk} + mc_{ic}\rho_{ic}$; $c\rho_{liq} = (1 - m)c_{sk}\rho_{sk} + mc_w\rho_w$; $\lambda_s = (1 - m)\lambda_{sk} + m\lambda_{ic}$; $\lambda_{liq} = (1 - m)\lambda_{sk} + m\lambda_w$; $a_{liq} = \lambda_{liq}/c\rho_{liq}$; $a_s = \lambda_s/c\rho_s$. Subscripts: sk, skeleton; ic, ice; w, water.

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