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MATHEMATICAL MODEL AND ALGORITHMS FOR AN ELECTRONIC COMPUTER ANALYSIS OF THE HEAT AND MASS TRANSFER IN FREEZING THE SOIL

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An analysis is performed of the selection of a mathematical model of the heat and mass transfer in freezing the soil, and an economical algorithm of its computation on an electronic computer is constructed.

Mathematical models of the heat and mass transfer during freezing disperse media can be separated into two groups [1]: in the first are models with a generalized Stefan-type condition on the moving interface of the thawed and frozen zones, while models without extraction of the freezing front with phase transitions in the whole volume are in the second.

The following assumption is ordinarily made in constructing the mathematical model of the first group: combined heat and mass transfer occurs in the thawed zone, while only heat transfer occurs in the frozen zone. Accordingly, the following system of equations [2] is used for the mathematical description of the freezing process:

$$c_{\text{т}} \frac{\partial T}{\partial t} = \operatorname{div}(\lambda_{\text{т}} \operatorname{grad} T), \tag{1}$$

$$\frac{\partial \omega_1}{\partial t} = \operatorname{div}(k \operatorname{grad} \omega_1), \tag{2}$$

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$$c_F \frac{\partial T}{\partial t} = \operatorname{div}(\lambda_F \operatorname{grad} T). \tag{3}$$

The second group of mathematical models of the freezing process is represented by a known system of heat- and mass-transfer equations of Lykov [3], which reduces for the case of capillary-porous bodies to the system of equations [4]:

$$c \frac{\partial T}{\partial t} = \operatorname{div}(\lambda \operatorname{grad} T) + \varepsilon L \gamma_0 \frac{\partial \omega_0}{\partial t}, \tag{4}$$

$$\frac{\partial \omega_0}{\partial t} = \operatorname{div}(k \operatorname{grad} \omega_0). \tag{5}$$

In this case the phase transformations are characterized by the parameter ε, the phase transformation criterion which is determined experimentally.

Application of the models mentioned in numerical investigations of freezing is fraught with definite difficulties related, particularly, to the necessity to give boundary conditions on the freezing front for the first model, and values of the criterion ε for the second. In this connection, papers [5, 6] have recently appeared in which modifications of the system (4) and (5) are used which do not contain the criterion ε. Thus, the following system of equations is used in [5]:

$$c \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(\lambda \frac{\partial T}{\partial x}\right) + L\rho_2 \frac{\partial \Phi}{\partial t}, \tag{6}$$

$$\frac{\partial \vartheta}{\partial t} = \frac{\partial}{\partial x}\left(D \frac{\partial \vartheta}{\partial x}\right) - \frac{\rho_2}{\rho_1} \frac{\partial \Phi}{\partial t}, \tag{7}$$

which describe heat and moisture transfer, respectively, with the phase transformation of water into ice taken into account.

A numerical investigation of the temperature and moisture fields around a borehole in permanently frozen mountain rock is performed in [6] on the basis of solving the following system of equations

$$c \frac{\partial T}{\partial t} = \operatorname{div}(\lambda (T) \operatorname{grad} T) + L\gamma_0 \frac{\partial}{\partial t}(i(T)\omega_0), \tag{8}$$

$$\frac{\partial \omega_0}{\partial t} = \operatorname{div}[k(\omega_0, T) \operatorname{grad}(1 - i(T))\omega_0]. \tag{9}$$

It is easy to note that systems (6)-(7) and (8)-(9) are equivalent; their sole difference is that the first system is written for the one-dimensional case and a volume content of moisture while the moisture content figures in the second. They can be represented in the form

$$c_{ef} \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(\lambda \frac{\partial T}{\partial x}\right) + L\gamma_0 \frac{\partial \omega_0^*}{\partial t}, \dagger \tag{10}$$

$$\frac{\partial \omega_0}{\partial t} = \frac{\partial}{\partial x}\left(k \frac{\partial \omega_1}{\partial x}\right), \tag{11}$$

where $c_{ef} = [c_0 + c_1\omega_H + c_2(\omega_0 - \omega_H) + L d\omega_H/dT]\gamma_0$; $\omega_0 = \omega_1 + \omega_2$ is the total moisture content.

Two algorithms for the numerical solution of system (10) and (11) are considered below, which correspond to two different representations of (11): the first algorithm is when (11) is replaced by the equation

$$\frac{\partial \tilde{\omega}}{\partial t} = \frac{\partial}{\partial x}\left(k \frac{\partial \tilde{\omega}}{\partial x}\right), \tag{12}$$

and the second corresponds to the case when its equivalent equation from [6] is taken in place of (11):

$$\frac{\partial \omega_0}{\partial t} = \frac{\partial}{\partial x}\left[k \frac{\partial}{\partial x}(1 - i(T))\omega_0\right]. \tag{13}$$

†The term with the asterisk acts only in the phase transition zone.

Equation (12) in the thawed zone agrees with (11) and expresses the change in moisture content in the liquid phase while it does not agree with it in the frozen zone and, therefore, describes the distribution of a certain fictitious moisture content. Starting from this, the algorithm for the numerical determination of the moisture field is developed so that this fictitious moisture content is first determined and then the moisture content in the liquid and solid phases is determined by using it and the known function ω_H.

The algorithm is constructed under the following initial and boundary conditions, although it can be considered under even more general conditions

$$\lambda \frac{\partial T}{\partial x} = \alpha (T - T_c),\ x = 0,\ t > 0, \tag{14}$$

$$\lambda \frac{\partial T}{\partial x} = 0,\ x = l,\ t > 0, \tag{15}$$

$$T(x,\ 0) = T^0(x),\ 0 \leqslant x \leqslant l,\ t = 0, \tag{16}$$

$$k \left.\frac{\partial \omega_0}{\partial x}\right|_{x=0} = k \left.\frac{\partial \omega_0}{\partial x}\right|_{x=l} = 0, \tag{17}$$

$$\omega_0(x,\ 0) = \omega^0(x),\ 0 \leqslant x \leqslant l,\ t = 0. \tag{18}$$

Taking account of the replacement of (11) by Eqs. (12) or (13), problem (10), (11), (14)-(18) is approximated on the difference mesh $\Omega = \{(x_i,\ t_j),\ x_i = ih,\ i = 0,\ 1,\ \ldots,\ N;\ Nh = l,\ t_j = \sum_{k=1}^{j} \tau_j\ \}$ by the following difference problem

$$c_{\mathrm{ef}\,ij}(T_{ij} - T_{ij-1})/\tau_j = [\lambda_{i+0.5j}(T_{i+1j} - T_{ij}) - \lambda_{i-0.5j}(T_{ij} - T_{i-1j})]/h^2 + \\ + L\gamma_0(\omega_{0,ij} - \omega_{0,ij-1})/\tau_j,\ i = 1,\ 2,\ \ldots,\ N-1;\ j = 1,\ 2,\ \ldots, \tag{19}$$

$$c_{\mathrm{ef},0j}(T_{0j} - T_{0j-1})/\tau_j = 2\lambda_{0.5j}(T_{1j} - T_{0j})/h^2 + 2\alpha(T_c - T_{0j})/h + L\gamma_0(\omega_{0.0j} - \omega_{0.0j-1})/\tau_j, \tag{20}$$

$$c_{\mathrm{ef},Nj}(T_{Nj} - T_{Nj-1})/\tau_j = -2\lambda_{N-0.5j}(T_{Nj} - T_{N-1j})/h^2 + L\gamma_0(\omega_{0,Nj} - \omega_{0,Nj-1})/\tau_j, \tag{21}$$

$$T_{i0} = T_i^0,\ i = 0,\ 1,\ \ldots,\ N, \tag{22}$$

$$(W_{ij} - W_{ij-1})/\tau_j = [k_{i+0.5j}(\eta_{i+1j} - \eta_{ij}) - k_{i-0.5j}(\eta_{ij} - \eta_{i-1j})]/h^2, \\ i = 1,\ 2,\ \ldots,\ N-1;\ j = 1,\ 2,\ \ldots, \tag{23}$$

$$(W_{0j} - W_{0j-1})/\tau_j = 2k_{0.5j}(\eta_{1j} - \eta_{0j})/h^2, \tag{24}$$

$$(W_{Nj} - W_{Nj-1})/\tau_j = -2k_{N-0.5j}(\eta_{Nj} - \eta_{N-1j})/h^2, \tag{25}$$

$$W_{i0} = \omega_i^0,\ i = 0,\ 1,\ \ldots,\ N, \tag{26}$$

where $W = \tilde{\omega}$, $\eta = \tilde{\omega}$ for the first algorithm, and $W = \omega_0$, $\eta = \omega_0(1 - i(T))$ for the second, while the coefficients λ, k, c_{ef} are calculated from the following formulas

$$\lambda_{i\pm0.5j} = \lambda(x_{i\pm0.5},\ t_j,\ 0.5(T_{in} + T_{i\pm1n}),\ 0.5(\omega_{0,in} + \omega_{0,i\pm1n})),$$

$$k_{i\pm0.5j} = k(x_{i\pm0.5},\ t_j,\ 0.5(T_{in} + T_{i\pm1n}),\ 0.5(\omega_{0,in} + \omega_{0,i\pm1n})),$$

$$c_{\mathrm{ef},ij} = [c_0 + c_1\omega_{H,in} + c_2(\omega_{0,in} - \omega_{H,in}) + L(d\omega_H/dT)_{in}]\gamma_0.$$

The derivative of the function $\omega_H(T)$ is calculated by starting from its analytical expression. We used the expression presented in [7] in this paper.

The subscript n in the formulas **for the coefficients** c_{ef}, λ, K takes on the values $n = j - 1$, j. For $n = j - 1$ the difference scheme (19)-(26) is a linear algebraic system whose solution is found by the factorization method, while a nonlinear system is obtained for $n = j$, for whose solution an iterative scheme is used. This scheme is written exactly the same as the system (19)-(26) except that their iterations must be taken in place of the unknowns T_{ij}, $\tilde{\omega}_{ij}$, $\omega_{o,ij}$, while the coefficients c_{ef}, λ, K are taken in the previous iteration.

FIRST ALGORITHM

Let values of the functions T_{ik}, $\omega_{o,ik}$, $\omega_{2,ik}$ be known for all $k = 0,\ 1,\ \ldots,\ j - 1$. To find them in the next time layer $t = t_j$ an iteration scheme is used. By means of the known

TABLE 1. Temperature Distribution T, Total Moisture ω_0 and Ice ω_2 over Depth of a Specimen of Sand Type for t = 50 h

	x	0,00	0,08	0,16	0,24	0,32	0,40	0,48	0,56	Counting time, sec
I	T	—10,17	—6,25	—2,39	0,65	2,59	4,26	5,65	6,77	2639
	ω_0	18,64	17,08	17,00	12,25	13,75	14,37	14,68	14,85	
	ω_2	17,64	16,01	14,83	0	0	0	0	0	
II	T	—10,24	—6,35	—2,47	0,58	2,54	4,20	5,59	6,73	2080
	ω_0	17,99	17,23	16,94	12,15	13,71	14,36	14,67	14,84	
	ω_2	16,99	16,17	14,82	0	0	0	0	0	
III	T	—10,20	—6,31	—2,44	0,59	2,55	4,22	5,61	6,74	1572
	ω_0	18,35	17,10	16,94	12,09	13,65	14,32	14,65	14,82	
	ω_2	17,35	16,05	14,80	0	0	0	0	0	
IV	T	—10,25	—6,37	—2,48	0,58	2,54	4,21	5,60	6,74	1438
	ω_0	17,99	17,08	16,89	12,11	13,67	14,33	14,65	14,82	
	ω_2	16,99	16,02	14,78	0	0	0	0	0	

$\overset{s}{T}_{ij}$, $\overset{s}{\omega}_{0,ij}$, the $\overset{s+1}{\tilde{\omega}}_{ij}$ is found from system (23)-(26), and then $\overset{s+1}{T}_{ij}$ from system (19)-(22). To find $\overset{s+1}{\omega}_0$, the $\overset{s+1}{\omega}_{1,ij}$, $\overset{s+1}{\omega}_{2,ij}$ are determined separately. Since the function $\omega_{1,ij}$ agrees with $\tilde{\omega}_{ij}$ in the thawed zone, but it is calculated in terms of a known function of the quantity of unfrozen water in the frozen zone, its s + 1 iteration is found in the whole domain of the solution from the relation

$$\overset{s+1}{\omega}_{1,ij} = \begin{cases} \overset{s+1}{\tilde{\omega}}_{ij}, & \overset{s+1}{T}_{ij} \geqslant 0, \\ \overset{s+1}{\omega}_{\text{H}}, & \overset{s+1}{T}_{ij} < 0. \end{cases}$$

Then the s + 1 iteration of the quantity $\overset{s+1}{\omega}_{2,ij}$ is calculated as the sum of the ice existing at the preceding time $\omega_{2,ij-1}$ and that newly formed because of the phase transformations

$$\overset{s+1}{\omega}_{2,ij} = \omega_{2,ij-1} + \overset{s+1}{\tilde{\omega}}_{ij} - \overset{s+1}{\omega}_{1,ij},$$

and from this latter stage we determine

$$\overset{s+1}{\omega}_0 = \overset{s+1}{\omega}_{1,ij} + \overset{s+1}{\omega}_{2,ij}.$$

SECOND ALGORITHM

Let the values of the functions T_{ik}, $\omega_{0,ik}$ be known for all k = 0, 1, ..., j − 1. Their determination on the time layer $t = t_j$ is performed by the same iteration scheme as for the case of the first algorithm. The difference is just that the iciness i(T) must be calculated in each iteration, i.e., the algorithm reduces to the following operations: From the known $\overset{s}{T}_{ij}$, $\overset{s}{\omega}_{0,ij}$, $i(\overset{s}{T}_{ij})$ the s + 1 iteration of the quantities T_{ij}, $\omega_{0,ij}$ are determined from the iteration scheme. Then $i(\overset{s+1}{T}_{ij})$ is calculated by using the known iciness function, and in the last stage we determine

$$\overset{s+1}{\omega}_{2,ij} = i(\overset{s+1}{T})\,\overset{s+1}{\omega}_{0,ij}, \quad \overset{s+1}{\omega}_{1,ij} = \overset{s+1}{\omega}_{0,ij} - \overset{s+1}{\omega}_{2,ij}.$$

Therefore, each of the algorithms permits finding the temperature distribution, the total moisture, and the moisture in the liquid and solid phases at any time.

Numerical computations were performed by means of the algorithms described under the following data

$$c_0 = 1180 \ \text{J/kg}\cdot\text{deg}, \qquad \gamma_0 = 1560 \ \text{kg/m}^3, \ L = 334\cdot 10^3 \ \text{J/kg},$$

$$\lambda(T,\ \omega_0) = 1{,}16\left[\lambda_{\text{F}} + (\lambda_{\text{T}} - \lambda_{\text{F}})\ \frac{\omega_{\text{H}}(T) - \omega_{\text{sand}}}{\omega_0 - \omega_{\text{sand}}}\right](\text{W/m}\cdot\text{deg}),$$

$$k(T,\ \omega_0) = k_1(T)\exp(k_2\omega_1 - k_3\omega_2)\ (\text{m}^2/\text{sec}),$$

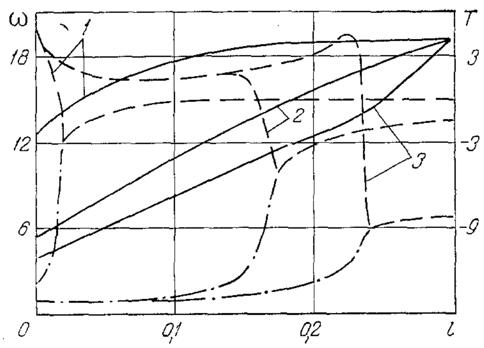

Fig. 1. Temperature distribution (solid line), total moisture content (dashes), and quantity of unfrozen water (dash-dot line) over specimen length at different times (t, h): 1) t = 2; 2) 24; 3) 72.

$$\lambda_{T,F} = m\ (0.001\gamma_0 + 0.1\omega_0 - 1.1) - 0.1\omega_0,$$

$$m_T = 1.5;\ m_F = 1.7;\ k_1(T) = 1.4\cdot 10^{-8}(1 + 0.04T),$$

$$k_2 = 0.172,\ \omega_{sand} = 1\%,\ l = 2.0\,\mathrm{m},\ h = 0.08,\ \tau = 180,$$

$$k_3 = 0.23, \alpha = 23.2\ \mathrm{W/m^2\cdot deg.}$$

Results of numerical computations are presented in the table: rows II, IV (I, III) correspond to computations by the first (second) algorithm, rows I, II (III, IV) by an implicit iteration (explicit) difference scheme.

Comparison of the corresponding values of the quantities T, ω_0, ω_2 computed by the two algorithms shows that the maximum discrepancy in the values of the temperature does not exceed 0.1°C, and 0.7% for the moisture. From a comparison of the machine time expenditure, it follows that the second algorithm requires ≈27% more time for the implicit scheme and 10% for the explicit scheme than for the first.

Therefore, it is expedient to use the first algorithm in practice, as being more economical. It should be expected that this advantage of the first algorithm will be still greater in solving multidimensional problems.

Results of a numerical computation by the first algorithm are presented in the figure for a specimen of length l = 0.3 m with the initial temperature T^0 = 4.2°C and with a boundary condition of the first kind for x = l: T(l, t) = 4.2°C. The data in the figure display the dynamics of a moisture change during freezing. It follows first from the figure that the moisture on the freezing front does not remain constant as is assumed when using the mathematical model of the first group, but decreases continuously as the freezing boundary moves into the bulk of the specimen.

Computations confirm the regularity established experimentally in the moisture distribution during freezing [8, 9]; an increase in moisture occurs within the whole freezing zone, and a diminution in the thawed zone; near the interface of the two zones a layer with the least moisture is observed.

NOTATION

x, spatial coordinate; t, time; T, temperature; c, c_T, c_F, volume specific heats of the soil, the thawed and the frozen soil; c_0, c_1, c_2, specific heats of the mineral skeleton, the water, and the ice; λ_T, λ_F, heat-conduction coefficients of the thawed and frozen soil; k(D), diffusion coefficient (moisture production); ρ_1, ρ_2, water and ice densities; γ_0, volume density of the skeleton; ϑ, Φ, volume content of the water and ice; ω_0, ω_1, ω_2, total moisture content, the moisture content in the liquid and solid phases; i(T), iciness; L, latent heat of melting of the ice; $\omega_H(T)$, function of the quantity of unfrozen water at the temperature T; α, heat elimination coefficient; T_C, temperature of the medium; $T^0(\omega_0)$, initial temperature (moisture content); l, specimen length; and h, τ_j, difference mesh spacings along the axes x and t.

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