MATHEMATICAL MODELING OF HEAT AND MASS TRANSFER PROCESSES IN GEOCRYOLOGICAL FORECASTS

P. P. Permyakov

UDC 551.345:536.421.001.57

A condition is found for the selection of a mathematical model of the temperature process and results are presented for the solution of the combined heat- and mass-transfer problem.

Confidence in the quantitative results of researches on the freezing–thawing of disperse media depends primarily on the selection of the mathematical model (MM). Many papers [1-7] are devoted to the mathematical modeling of this physical process but not all the proposed MM are applied extensively in practical geocryological forecasting. The reason for this is the lack of a functional dependence on the temperature and the total humidity of certain phenomenological parameters or boundary conditions (the coefficient of diffusion in the freezing–thawing zone, for instance) [5, 8, 9]. By using special methods of identification in recent years, new algorithms have been developed to restore the mentioned MM parameters of heat and mass transfer (HMT) [10, 11].

I. The general MM of the heat and moisture propagation process is given in freezing–thawing disperse media by the system of A. V. Lykov equations [1-3]

$$c\rho \frac{\partial T}{\partial \tau} = -\operatorname{div} \mathbf{q}_t + L \frac{\partial \rho \omega_i}{\partial \tau}, \quad (1)$$

$$\frac{\partial \rho \omega_w}{\partial \tau} = -\operatorname{div} \mathbf{q}_\omega - \frac{\partial \rho \omega_i}{\partial \tau}, \quad (2)$$

where $\mathbf{q}_t = -\lambda \operatorname{grad} T + c_w T \mathbf{q}_\omega$; $\mathbf{q}_\omega = -k\rho(\operatorname{grad} \omega_w + \delta \operatorname{grad} T)$; $\mathbf{q}_t$, $\mathbf{q}_\omega$ are vectors of the specific thermal and moisture flux densities (W/m², kg/(m²·sec)).

For simplicity in the exposition we consider a one-dimensional seasonal freezing–thawing problem for a moist disperse material. Two approaches (kinds) of interpretation are known at the present time for the above-mentioned MM of HMT [6].

1. In coarse dispersed media the phase transition of free water occurs completely at the specific temperature $T_f = 273°K$. Such a jumplike change in the aggregate state of free water takes into account the balance condition on the moving phase separation boundary $\xi(\tau)$. The temperature fields in the frozen and thawed zones are described, respectively, by the usual heat-conduction equations [1, 6]. The moisture ω_w migrates only in the thawed zone.

The following conditions are satisfied on the moving phase interface $\xi(\tau)$: a Stefan-type condition is conserved for the heat fluxes

$$\lambda_m \frac{\partial T_m}{\partial x}\Big|_{\xi^-} - \lambda_t \frac{\partial T_t}{\partial x}\Big|_{\xi^+} - L\rho k \frac{\partial \omega_w}{\partial x} = L\rho(\omega_w - \omega_{gr}) \frac{\partial \xi}{\partial \tau}, \quad (3)$$

and the continuity condition for the temperature

$$T_m(\xi^-, \tau) = T_t(\xi^+, \tau) = T_f = \text{const}. \quad (4)$$

Without taking account of the moisture transfer ω_w we later denote the temperature problem, also known as the Stefan problem, by MM TP-1, and the combined heat- and mass-transfer problem by MM HMT-1.

Institute of Physicotechnical Problems of the North, Yakutsk Branch, Academy of Sciences of the USSR. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 53, No. 1, pp. 124-129, July, 1987. Original article submitted March 4, 1986.

 0022-0841/87/5301-0840$12.50 © 1988 Plenum Publishing Corporation

TABLE 1. Parameters of the Nonfrozen Water Functions

Rock	a	b	d	ω^0, %	A, %	ω_{gr}, %	T_1, K	T_2, K	T_3, K
Gravel	4,1	0,73	0,00	15	6,8	1,11	267	272,5	273
Siltstone	11,73	0,80	0,33	5	5,0	1,40	253	269,84	269,84
Limestone	1,78	0,90	1,44	5	2,4	1,60	253	271,00	273

2. Different salty and finitely dispersed media are characterized by certain freezing–thawing singularities. The free water in these media freezes at a temperature of $T_f = 273°K$ while the bound water is crystallized as the temperature is lowered [3, 6, 12]. A change in the aggregate state of the bound water occurs in a certain temperature band $[T_1, T_2]$ (Table 1) whereupon a freezing zone is formed. The MM HMT-2 has the form [2, 4-6]

$$c\rho \frac{\partial T}{\partial \tau} = \frac{\partial}{\partial x}\left(\lambda \frac{\partial T}{\partial x}\right) + L \frac{\partial \rho\omega_i}{\partial \tau}, \tag{5}$$

$$\frac{\partial \rho\omega_w}{\partial \tau} = \frac{\partial}{\partial x}\left(k \frac{\partial \rho\omega_w}{\partial x}\right) - \frac{\partial \rho\omega_i}{\partial \tau}, \tag{6}$$

$$0 < x < l, \quad \tau > 0.$$

For simplicity in the subsequent exposition we isolate the MM of the temperature problem (5) and denote it by MM TP-2. We first examine the question of mathematical modeling of the temperature process.

II. The degree of thawing–freezing $\xi(T)$ is ordinarily of interest for geocryological forecasting. The degree of thawing for the MM TP-1 is determined by the temperature isotherm $T_f = 273°K$, while the concept of the thawing–freezing front is missing for the MM TP-2 since the phase transition of the interstitial water occurs in a certain temperature band. In order to select the degree of thawing $\xi(T)$ for the MM TP-2 we first consider the physical considerations from which the phase transition temperature T_f is selected for the MM TP-1.

The Stefan problem (MM TP-1) is ordinarily solved numerically by a smoothing method [13]. This is equivalent to the assumption that the phase transition occurs in a certain temperature interval whose length is determined by the magnitude of the smoothing parameter Δ and not at one definite temperature T_f. Different values of this parameter are usually given in a numerical experiment, i.e., the phase transition temperature band is changed and the power of the phase transition heat source remains constant. It should be noted that $T_f = 273°K$ is the mean temperature of the phase transition heat source T_f^m and the temperature at which equality of the quantity (mass) of water in the solid (ice) and liquid (water) state $T_{i.w.}$ is observed, i.e., $T_f = T_f^m = T_{i.w.} = 273°K$.

For the MM TP-2 these temperatures are expressed in terms of the function of the quantity of nonfreezing water $\omega_{n.w.}(T)$:

$$T_f^m = \frac{1}{\omega^0 - \omega_{gr}} \int_{T_1}^{T_3} T \frac{\partial \omega_{n.w}(T)}{\partial T} dT,$$

$$T_{i.w.} = \omega_{n.w.}^{-1}((\omega^0 - \omega_{gr})/2).$$

The isotherms of these temperatures $\xi(T_f^m)$, $\xi(T_{gr})$ may be taken as the thawing–freezing front for the MM TP-2. For any disperse medium the T_f^m, $T_{i.w.}$ do not usually agree (see Table 3 below).

Taking account of the above-mentioned temperatures T_f^m and $T_{i.w.}$, numerical computations are performed for two different boundary conditions

$$\lambda \frac{\partial T}{\partial x}\bigg|_{x=l} = 0, \quad \tau > 0, \tag{I}$$

$$T|_{x=l} = T^0, \quad \tau > 0. \tag{II}$$

TABLE 2. Thermophysical Characteristics of Rocks

Rock	$c_{ск}$, J/(kg·K)	ω^0, %	λ_t, W/(m·K)	λ_m, W/(m·K)	ρ, kg/m³
Gravel	748,8	5	1,16	1,39	1600
Same	748,8	10	1,33	1,80	1600
»	748,8	15	1,74	2,21	1600
»	748,8	20	2,04	2,72	1600
Siltstone	874,4	5	1,80	2,07	2400
Limestone	852,8	5	2,50	3,13	2400

TABLE 3. Degrees of Thawing ξ(T) (m), Obtained by Using Different MM

Rock, number	ω^0, %	T_f^m, K	$T_{1,w}$ K	$\xi(T_f)$, TP-1	$\xi(T_f)$, TP-2	$\xi(T_{1,w})$, TP-2	$\xi(T_w^m)$, TP-2	$\xi(T_{1,w})$, TP-1	$\xi(T_f^m)$, TP-1	ξ, HMT-2 $(\omega_1 \approx \omega_w)$	$\xi(T_f^m)_{TP-2} - \xi(T_f)_{TP-1}$
Gravel											
I	5	270,9	271,0	2,15	2,50	8,30	9,50	8,67	9,00	7,75	7,35
II	5	270,9	271,0	2,10	2,20	5,20	5,65	5,31	5,95	4,80	3,55
I	10	271,9	272,3	1,70	1,50	2,25	2,85	2,15	2,40	1,90	1,15
II	10	271,9	272,3	1,60	1,52	2,10	2,60	2,19	2,30	1,90	1,00
I	15	272,2	272,5	1,55	1,35	1,75	2,25	1,83	2,00	1,50	0,70
II	15	272,2	272,5	1,50	1,20	1,60	2,00	1,68	1,80	1,50	0,50
II	20	272,5	272,75	1,34	1,20	1,42	1,55	1,46	1,58	1,35	0,21
II	20	272,6	272,76	1,35	1,30	1,42	1,50	1,43	1,45	1,35	0,15
Limestone											
I	5	271,1	271,2	2,75	2,85	T*	—	—	—	—	—
II	5	271,1	271,2	2,40	2,50	5,10	5,40	5,43	5,60	—	3,00
Siltstone											
I	5	265,5	264,8	2,45	4,90	T	—	—	—	—	—
II	5	265,5	264,8	2,10	3,75	T	—	—	—	—	—

*Specimen in the thawed state.

Taken as initial data for the model example were: $-\lambda \left.\frac{\partial T}{\partial x}\right|_{x=0} = \alpha(T - T_c(\tau))$, $\tau > 0$; $T(x, 0) = T^0$, $0 \le x \le l$; $T_c(\tau) = A_0 - A_1 \cos(2\pi(\tau - \tau_1)/\tau_2)$; $A_0 = 273$ K; $A_1 = 6$ K; $\tau_1 = 131.4 \cdot 10^4$ sec; $\tau_2 = 315.36 \cdot 10^5$ sec; $\Delta\tau = 525.6 \cdot 10^3$ sec; $\alpha = 8.715$ W/(m²·K); $N = 40$; $T^0 = 269$ K.

The thermal properties and parameters of the nonfrozen water of soils are represented in Tables 1 and 2 [9, 10]. The problems described numerically were solved on an electronic computer by an implicit difference scheme with the use of iteration [13].

Presented in Table 3 are the degrees of seasonal thawing at the end of September after 5 years, computed by using different MM.

It is seen from the numerical experiment that upon satisfying the inequality $|T_f - T_f^m| < 0.5$°K the maximal discrepancy in the degree of thawing $\Delta\xi$ does not exceed 15% ($\Delta\xi$ is the relative error in the degree of thawing

$$\Delta\xi = \frac{|\xi(T_f) - \xi(T_f^m)|}{\xi(T_f^m)} 100, \ \%,$$

$\xi(T_f)$, $\xi(T_f^m)$ are the isotherms of the temperatures T_f and T_f^m obtained by using the MM TP-1 and TP-2, respectively).

It hence follows that in coarsely dispersed media where the bound water content is slight $|T_f - T_f^m| < 0.5$°K and $[T_1, T_3] \subset [T^0, T_c]$, it is expedient to use MM TP-1 (the Stefan formulation). The quantity 0.5°K is found as a result of analyzing the solutions of heat conduction problems obtained by using the two considered MM [6, 14, 15]. In the opposite case ($|T_f - T_f^m| \ge 0.5$°K) it is necessary to use MM TP-2 for an accurate forecast of the temperature field. The confidence of such an approach follows from the fact that the divergence of the isotherms $\xi(T_f)$ and $\xi(T_f^m)$ (Table 3) grows as the difference $|T_f - T_f^m|$ increases.

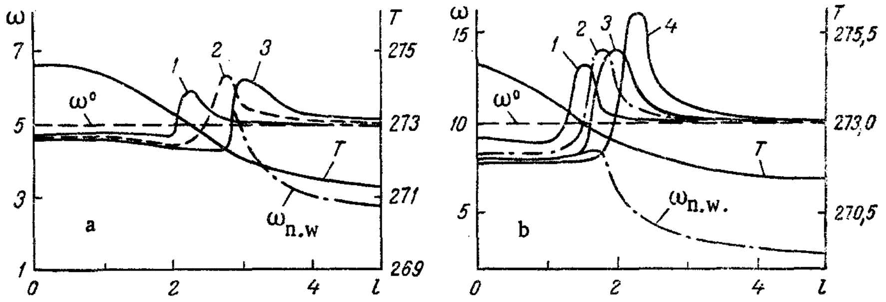

Fig. 1. Distribution of the temperature T and nonfrozen water $\omega_{n.w.}$ along the specimen length for $\tau = 5$ years ($a - \omega^\circ = 5\%$; b — 10) and change in the total humidity ω at different times: 1) 1 year; 2) 3; 3) 5; 4) 10. ω, %; T, K; l, m.

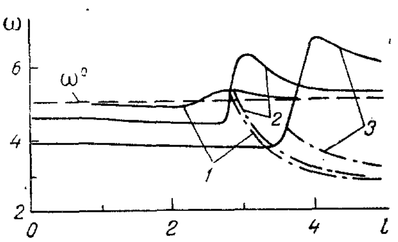

Fig. 2

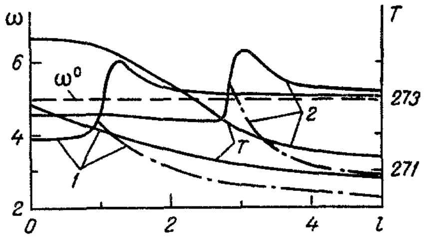

Fig. 3

Fig. 2. Dynamics of the distribution of the total humidity ω (solid lines) and the nonfrozen water $\omega_{n.w}$ (dash-dot) for different values of the diffusion coefficient: 1) 0.1 k; 2) 1 k; 3) 10 k.

Fig. 3. Profile of the total humidity ω, temperature T, and nonfrozen water $\omega_{n.w}$ (dash-dot lines) along the specimen length: 1, 2) with and without taking account of heat insulation.

If there is no requirement of high accuracy on the computation then MM TP-1 can be used. Here $T_{i.w.}$ or T_f^m can be taken here as the phase transition temperature T_f (see Table 3). Such a shift of the phase transition point results in approximation of the temperature fields calculated by using MM TP-1 and TP-2, and permits an approximately 20% saving in machine time as compared with the MM TP-2. It should also be noted that the limestone (I) and siltstone (I, II) specimens are in the thawed state according to MM TP-2 while the degrees of thawing do not go beyond the limits 2.75 m (Table 3) according to MM TP-1.

III. After the identification of the missing coefficients [10] in the mathematical modeling of combined heat- and mass-transfer processes, MM TP-2 is extensively applied in practice.

Presented in Figs. 1a and b are results of a numerical experiment of the mentioned process at the end of September, obtained by using the MM HMT-2 at different times for a closed specimen with respect to humidity, i.e.,

$$k\left.\frac{\partial\rho\omega_w}{\partial x}\right|_{x=0} = k\left.\frac{\partial\rho\omega_w}{\partial x}\right|_{x=l} = 0.$$

The initial data of the temperature problem is from Sec. 2. The initial humidity equals $\omega^\circ = 5$, 10%. We represent the diffusion coefficient in the form $k = k(T, \omega_w, \omega_i) = k_1(T) \exp(k_2\omega_w - k_3\omega_i)$, m²/sec, $k_1(T) = 1.4 \cdot 10^{-8}(1 + 0.04T)$; $k_2 = 0.172$; $k_3 = 0.23$.

It is seen from Fig. 1 that migration of the interstitial water towards the frozen zone is observed in the first year of the temperature action. In subsequent years the migration of the nonfrozen moisture is magnified and moves toward the frozen zone. As ω° increases the maximal value of the total humidity grows, which can result in an abrupt change in the strength and deformation properties of the dispersed rock.

Shown in Fig. 2 are graphs of the distribution of the total humidity ω along the specimen length at the end of September (after 5 years) for different values of the diffusion coefficient. In the third case the diffusion coefficient is 10 times greater than in the second and the process of moisture tending toward the frozen zone is magnified, the zone of shrinkage and the degree of thawing increase, correspondingly, by 30-40%.

Presented in Fig. 3 is a comparison between the distributed temperature T and the total humidity ω obtained with and without the heat insulation coating on the left boundary of the disperse medium taken into account at the end of September after 5 years. Polyurethane foam PPU-6 of 0.1 m thickness was taken as heat insulation. It is seen from the figure that application of a heat shield coating reduces the degree of thawing, diminishes the tendency of the total humidity toward the freezing zone. It hence follows that heat insulating material can be used to control the strength and deformation properties of frozen disperse rocks [16, 17].

NOTATION

c, specific heat; k, diffusion coefficient; L, specific heat of the phase transition; l, plate thickness; N, number of sites in the spatial coordinate; T, temperature; A_0, A_1, T_1, T_2, T_3, constant temperatures; T_C, external temperature; ω_i, ω_l, $\omega_{n.w}$, ω_{gr}, ω, ice, water, and nonfrozen, securely bound, and total humidity; x, spatial coordinate; α, heat elimination coefficient; $\Delta\tau$, time step in the mesh; τ_1, τ_2, constant times; δ, thermal gradient coefficient; ξ, location of the phase transition front; λ, heat conduction coefficient; τ, time; ρ, bulk density of the mineral skeleton. Subscripts: m, frozen; t, thawed; 0, initial; w, water; i, ice.

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