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NUMERICAL-ANALYTIC ALGORITHM OF THE STEFAN PROBLEM SOLUTION

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An algorithm is developed for the numerical solution of the Stefan problem for boundary conditions of the first, second, and third kinds, respectively, on the surface of a freezing (thawing) layer by using the solution of the heat conduction equation in the form of a series in the spatial coordinate including two derivatives of the time functions and their derivatives. An approximate estimation of the proposed method is given in an example of computing the freezing of water in a reservoir.

The necessity to determine the temperature state of objects being investigated with the natural-time change in the environment and the parameters governing it taken into account (the wind velocity, solar radiation, snow cover) occurs in solving many practical problems of engineering glaciology, geocryology, and metallurgy. Determination of the phase transition front of freezing water, soil, or a cooling metal ingot in a general formulation is a complex problem whose methods of solution still remain largely undeveloped [1-3]. This refers mainly to multidimensional problems with moving boundaries and one-dimensional problems with boundary conditions different from the first kind. Boundary conditions of the first kind for which the solution of the Stefan problem has been developed sufficiently completely assume the temperature of the surface of the freezing (thawing) massif to be given. In practice this yields results that are only qualitatively in agreement with the actual process. The algorithm considered below for the solution does not impose similar constraints and is similar in its content to the method of differential series [4, 5] but differs favorably from the latter in its clearness and simplicity. The formulated problem can be solved for any boundary conditions by an insignificant modification of one formula. Moreover, the temperature field of the freezing (thawing) or cooling layer needed for stress state computations and the motion law $\xi(\tau)$ of the phase interface boundary can be determined. The mathematical formulation of the problem has the form

$$\frac{\partial t_1(x,\ \tau)}{\partial \tau} = a_1 \frac{\partial^2 t_1(x,\ \tau)}{\partial x^2},\ x \in [0,\ \xi(\tau)],\ \tau \in [0,\ \infty], \tag{1}$$

$$\frac{\partial t_2(x,\ \tau)}{\partial \tau} = a_2 \frac{\partial^2 t_2(x,\ \tau)}{\partial x^2},\ x \in [\xi(\tau),\ \infty],\ \tau \in [0,\ \infty], \tag{2}$$

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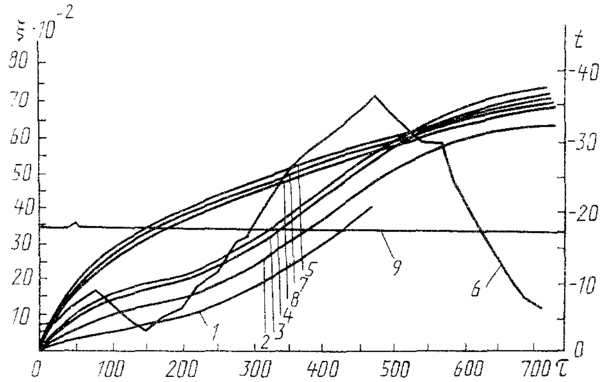

Fig. 1. Graphs of the degree of water freezing in time: 1, 2, 3) for boundary conditions of the third kind $\alpha(\tau)$ = 11.63; 23.26, and 116.3 W/(m^2·K), respectively; 4) for boundary conditions of the first kind corresponding to the real behavior of the temperature variation; 5) for boundary conditions of the first kind corresponding to the mean-monthly temperature; 6) outside air temperature change in time; 7) degree of freezing calculated from (31); 8) self-similar solution of the Stefan problem; 9) mean-monthly temperature. ξ, m; t, °C; τ, g.

with boundary conditions on the surface of the freezing (thawing) massif:

First kind

$$t_1(0, \tau) = t_{sur}(\tau), \ \tau \in [0, \infty], \tag{3}$$

Second kind

$$\lambda_1 \frac{\partial t_1(x, \tau)}{\partial x}\bigg|_{x=0} = q_{sur}(\tau), \ \tau \in [0, \infty], \tag{4}$$

Third kind

$$\lambda_1 \frac{\partial t_1(x, \tau)}{\partial x}\bigg|_{x=0} = \alpha(\tau)[t_m(\tau) - t_1(0, \tau)], \ \tau \in [0, \infty], \tag{5}$$

on the moving phase interface boundary for $x = \xi(\tau)$

$$t_1(\xi(\tau), \tau) = t_2(\xi(\tau), \tau) = t_p; \tag{6}$$

$$\lambda_1 \frac{\partial t_1(x, \tau)}{\partial x}\bigg|_{x=\xi(\tau)-0} - \lambda_2 \frac{\partial t_2(x, \tau)}{\partial x}\bigg|_{x=\xi(\tau)+0} = q_p \frac{d\xi(\tau)}{d\tau}; \tag{7}$$

$$\xi(0) = 0, \tag{8}$$

for equation (2)

$$\frac{\partial t_2(x, \tau)}{\partial x}\bigg|_{x\to\infty} = 0, \ \tau \in [0, \infty], \tag{9}$$

with the initial condition

$$t_2(x,\ 0) = \Theta_2(x),\ x \in [0,\ \infty]. \tag{10}$$

The law of phase interface boundary motion $\xi(\tau)$ with (8) taken into account assumes that the domain of definition of (1) is concentrated for $\tau = 0$ at a point (is degenerate) and consequently the initial conditions is taken equal to zero. Formulation of condition (8) in the form in which it is taken is limited from the representation of the solution of (1) in spatial coordinates in the form of a power series including two arbitrary time function $\varphi(\tau)$ and $\Psi(\tau)$ and their derivatives that are later determined as a function of the boundary conditions from (3)-(5) and (6):

$$t_1(x,\ \tau) = \sum_{n=0}^{\infty} \left\{ \frac{x^{2n}}{a_1^n 2n!} \left[\left(\frac{d}{d\tau} \right)^n \varphi(\tau) \right] + \frac{x^{2n+1}}{a_1^n (2n+1)!} \left[\left(\frac{d}{d\tau} \right)^n \Psi(\tau) \right] \right\}, \tag{11}$$

It is characteristic for the solution of (11) that for $\tau \in [0, \infty]$

$$t_1(0,\ \tau) = \varphi(\tau),\quad \left. \frac{\partial t_1(x,\ \tau)}{\partial x} \right|_{x=0} = \Psi(\tau).$$

Upon their substitution into conditions (3)-(5) we obtain the following expressions

$$\varphi(\tau) = t_{\text{sur}}(\tau),\ \tau \in [0,\ \infty], \tag{12}$$

$$\Psi(\tau) = q_{\text{sur}}(\tau)/\lambda_1,\ \tau \in [0,\ \infty], \tag{13}$$

$$\varphi(\tau) = \frac{\lambda_1}{\alpha(\tau)} \Psi(\tau) + t_{\text{m}}(\tau),\ \tau \in [0,\ \infty], \tag{14}$$

that must be used as relationships governing the interconnection between the functions $\varphi(\tau)$ and $\Psi(\tau)$ and their derivatives as a function of the boundary conditions on the surface of the medium under investigation. Upon satisfaction of (11), condition (6) on the moving boundary and taking account of (12)-(14) to determine the function $\Psi(\tau)$ (for boundary conditions of the first and third kinds) and $\varphi(\tau)$ (for the boundary condition of the second kind), we obtain the following differential equation:

For boundary conditions of the first kind (3) with (12) taken into account

$$t_{\text{p}} = \sum_{n=0}^{\infty} \left\{ \frac{(\xi(\tau))^{2n}}{a_1^n 2n!} \left[\left(\frac{d}{d\tau} \right)^n t_{\text{sur}}(\tau) \right] + \frac{(\xi(\tau))^{2n+1}}{a_1^n (2n+1)!} \left[\left(\frac{d}{d\tau} \right)^n \Psi(\tau) \right] \right\}, \tag{15}$$

For boundary conditions of the third kind (5) with (14) taken into account

$$t_{\text{p}} = \sum_{n=0}^{\infty} \left\{ \left[\frac{(\xi(\tau))^{2n} \lambda_1}{a_1^n 2n!\ \alpha(\tau)} + \frac{(\xi(\tau))^{2n+1}}{a_1^n (2n+1)!} \right] \left[\left(\frac{d}{d\tau} \right)^n \Psi(\tau) \right] + \frac{(\xi(\tau))^{2n}}{a_1^n 2n!} \left[\left(\frac{d}{d\tau} \right)^n t_{\text{cp}}(\tau) \right] \right\}, \tag{16}$$

For boundary conditions of the second kind (4) with (13) taken into account

$$t_{\text{p}} = \sum_{n=0}^{\infty} \left\{ \frac{(\xi(\tau))^{2n}}{a_1^n 2n!} \left[\left(\frac{d}{d\tau} \right)^n \varphi(\tau) \right] + \frac{(\xi(\tau))^{2n+1}}{\lambda_1 a_1^n (2n+1)!} \left[\left(\frac{d}{d\tau} \right)^n q_{\text{sur}}(\tau) \right] \right\}. \tag{17}$$

If we take

$$\Psi(\tau) = (t_{\text{p}} - t_{\text{sur}}(\tau))/\xi(\tau); \tag{18}$$

$$\frac{d^n \Psi(\tau)}{d\tau^n} = -\left[\left(\frac{d}{d\tau} \right)^n t_{\text{sur}}(\tau) \right] (2n+1)/\xi(\tau), \tag{19}$$

then (15) is transformed into an identity. This confirms that (18) and (19) are the solution of (15). Analogous relationships hold for (16) for

$$\Psi(\tau) = (t_p - t_m(\tau)) \Big/ \left(\xi(\tau) + \frac{\lambda_1}{\alpha(\tau)} \right); \tag{20}$$

$$\frac{d^n \Psi(\tau)}{d\tau^n} = -\left[\left(\frac{d}{d\tau} \right)^n t_m(\tau) \right] \Big/ \left(\frac{\lambda_1}{\alpha(\tau)} + \frac{\xi(\tau)}{(2n+1)} \right), \tag{21}$$

as well as for (17) for

$$\varphi(\tau) = t_p - \frac{\xi(\tau)}{\lambda_1} q_{sur}(\tau), \tag{22}$$

$$\frac{d^n \varphi(\tau)}{d\tau^n} = -\frac{\xi(\tau)}{\lambda_1(2n+1)} \left[\left(\frac{d}{d\tau} \right)^n q_{sur}(\tau) \right]. \tag{23}$$

If the change in the derivatives of the function $\Psi(\tau)$ with respect to time are neglected in (18) and (19) then they are formulas to determine the heat flux to the freezing front used for the approximate solution of the Stefan problem [2], which is a confirmation of the more general nature of the results obtained.

For known values of the functions $\varphi(\tau)$ and $\Psi(\tau)$ determined by the solution of the differential equations (15)-(17), the heat flux to the freezing (thawing) front should be determined in the general case from the expression

$$\lambda_1 \frac{\partial t_1(x, \tau)}{\partial x} \bigg|_{x=\xi(\tau)} = \lambda_1 \left[\sum_{n=1}^{\infty} \frac{(\xi(\tau))^{2n-1}}{a_1^n (2n-1)!} \left[\left(\frac{d}{d\tau} \right)^n \varphi(\tau) \right] + \sum_{n=0}^{\infty} \frac{(\xi(\tau))^{2n}}{a_1^n 2n!} \left[\left(\frac{d}{d\tau} \right)^n \Psi(\tau) \right] \right]. \tag{24}$$

Using the relationships (18)-(23), we determine the heat flux satisfying the given boundary condition in each specific case from (24). The heat flux directed toward the freezing front from the thawed zone and corresponding to the solution (2) in the domain $\Omega_2 = \{x \geq \xi(\tau), \tau \in [0, \infty]$ for $\Theta_2(x) = t_2 = \text{const}$, is found from the dependence that is ordinarily utilized for approximate and self-similar solutions of the Stefan problem [2, 6]:

$$\lambda_2 \frac{\partial t_2(x, \tau)}{\partial x} \bigg|_{x=\xi(\tau)+0} = \frac{\lambda_2 t_2}{\sqrt{\pi a_2 \tau}}, \quad \tau \in [0, \infty]. \tag{25}$$

Taking account of (24) and (25), we obtain from condition (7):

For boundary conditions for the first kind

$$\frac{dy}{d\tau} = \frac{2}{q_p} \left\{ \lambda_1 \left[\sum_{n=1}^{\infty} \frac{y^n}{a_1^n (2n-1)!} \left[\left(\frac{d}{d\tau} \right)^n t_{sur}(\tau) \right] + t_p - t_{sur}(\tau) + \sum_{n=1}^{\infty} \frac{y^n (2n+1)}{a_1^n 2n!} \left[\left(\frac{d}{d\tau} \right)^n t_{sur}(\tau) \right] \right] - \sqrt{y} \lambda_2 \frac{t_2}{\sqrt{\pi a_2 \tau}} \right\}, \tag{26}$$

For boundary conditions of the second kind

$$\frac{dy}{d\tau} = \frac{2}{q_p} \left\{ \lambda_1 \left[\sum_{n=1}^{\infty} \frac{y^{n-\frac{1}{2}}}{a_1^n (2n-1)!} \left(-\frac{2na_1}{\lambda_1} \right) \left[\left(\frac{d}{d\tau} \right)^n q_{sur}(\tau) \right] + \frac{\sqrt{y} q_{sur}(\tau)}{\lambda_1} + \sum_{n=1}^{\infty} \frac{y^{n+\frac{1}{2}}}{a_1^n 2n! \lambda_1} \left[\left(\frac{d}{d\tau} \right)^n q_{sur}(\tau) \right] \right] - \sqrt{y} \lambda_2 \frac{t_2}{\sqrt{\pi a_2 \tau}} \right\}, \tag{27}$$

For boundary conditions of the third kind

$$\frac{d\xi(\tau)}{d\tau} = \frac{1}{q_m} \left\{ \lambda_1 \left[\sum_{n=1}^{\infty} \left(\frac{\lambda_1}{\alpha(\tau)} \frac{(\xi(\tau))^{2n-1}}{a_1^n (2n-1)!} + \frac{(\xi(\tau))^{2n}}{a_1^n 2n} \right) \left[\left(\frac{d}{d\tau} \right)^n \Psi(\tau) \right] + \Psi(\tau) + \sum_{n=1}^{\infty} \frac{(\xi(\tau))^{2n-1}}{a_1^n (2n-1)!} \left[\left(\frac{d}{d\tau} \right)^n t_m(\tau) \right] \right] - \lambda_2 \frac{t_2}{\sqrt{\pi a_2 \tau}} \right\}. \tag{28}$$

The equations obtained are nonlinear in the degree of freezing (thawing) in all the boundary conditions considered. The Runge—Kutta method of its modification [7] is a sufficiently well-developed method for the approximate solution of such equations.

The surface temperature $t_{surf}(\tau)$, the heat flux $q_{surf}(\tau)$ and the environment temperature $t_m(\tau)$, that should be represented in the form of analytic dependences in the solution, all enter into (26)-(28). The mentioned characteristics are determined discretely at definite time intervals during the day in the practice of meteorological observations. It is necessary to select an analytic dependence from these data which would be the best approximation to the given one. Let values of the temperature determined after different time intervals τ_k during a time interval L be known. For instance $\tau_m(\tau)_k = (t_m)_k = t_k$; ($k = 0, 1, 2, ..., 2p$), then the sum

$$t_m(\tau) = \frac{a_0}{2} + \sum_{m=1}^{p} \left(a_m \cos m \frac{2\pi\tau}{L} + b_m \sin m \frac{2\pi\tau}{L} \right) \tag{29}$$

will be the best approximation of the given discrete temperature distribution if the coefficients a_0, a_m, and b_m are calculated from the formulas [8]

$$a_0 = \frac{1}{p} \sum_{k=0}^{2p-1} t_k; \quad a_m = \frac{1}{p} \sum_{k=0}^{2p-1} t_k \cos \frac{km\pi}{p}; \quad b_m = \frac{1}{p} \sum_{k=0}^{2p-1} t_k \sin \frac{km\pi}{L};$$

$m = 1, 2, 3, ...,$ where $b_p = 0$. The derivatives with respect to time of (29) needed in the computations are here determined as

$$\frac{d^n t_m(\tau)}{d\tau^n} = \sum_{m=1}^{p} \left(\frac{2\pi m}{L} \right)^n \left[a_m \left(\cos \left(m \frac{2\pi\tau}{L} + \frac{n\pi}{2} \right) \right) + b_m \left(\sin \left(m \frac{2\pi\tau}{L} + \frac{n\pi}{2} \right) \right) \right]. \tag{30}$$

The temperature determined by means of (29) will equal the surface temperature of the freezing massif if appropriate measurings of the temperature on the surface are used in determining the coefficients a_0, a_m, and b_m. The heat flux is determined in an analogous manner. The solution of the differential equations (26)-(28) with (18)-(23), (29), and (30) taken into account was realized by a Runge—Kutta method of fourth order of accuracy on an electronic computer. The problem was solved in application to the formation of ice in a reservoir in the fall. The values of the quantities entering into the computation are $\lambda_1 = 1.97$ W/(m·K); $\lambda_2 = 0.58$ W/(m·K); $\xi(0) = 0$; $a_1 = 0.00378$ m²/h; $a_2 = 0.0005$ m²/h; $t_2 = 2.4$°C; $q_p = 335200$ kJ/m³; $t_p = 0$°C; $L = 720$ h; $p = 15$.

One of the modifications using the mean monthly temperature ($t_1 = -17.1$°C) was solved with boundary conditions corresponding completely to the solution of the self-similar problem [2]. In this case the regularity of the change in degree of freezing agreed completely with the computations performed according to the known formula $\xi(\tau) = \beta\sqrt{\tau}$ (Fig. 1, curves 5, 7, 8). The results practically agree if β is determined from the formula [2]

$$\beta = \sqrt{\mp \frac{2\lambda_1 t_1}{q_p} + \frac{\lambda_2 t_2^2}{\pi a_2 q_p^2}} \mp \frac{t_2}{g_p} \sqrt{\frac{\lambda_2}{\pi a_2}}, \tag{31}$$

and differ by less than 3% for β determined from the rigorously self-similar solution. A certain difference between them is apparently due to just the error in the approximation of the constant mean-monthly temperature (curve 9) according to (29). On the whole, the consistent agreement between these three results in the whole range of computed time variation with an error not exceeding 3% is one of the proofs of the correctness of the method developed.

Upon using the real behavior of the outside air temperature variation (curve 6) in the computations, the degree of freezing determined by the computation differs, in principle, from the self-similar solution by times up to 50% (curves 4 and 5). The influence of the temperature change appears especially substantially for small values of the degree of freezing ($\xi(\tau) < 0.5$ m). As the thermal resistance of the frozen layer increases, this influence is smoothed out. Among the physical phenomena increasing the thermal resistance of the frozen layer is also the state of its surface, for instance, the presence of snow cover and the change in the surface heat transfer coefficient to a near-earth air layer. In the most simple case these processes can be taken into account in approximate engineering computations by the following expression

$$\alpha_{ef}(\tau) = \frac{1}{1/\alpha(\tau) + \delta_{sn}(\tau)/\lambda_{sn}(\tau)}.$$

The substantial influence of the air heat transfer coefficient to the surface on the magnitude of the freezing (curves 1, 2, 3) was detected in the 11.63-116.3 W/(m^2·K) range by computations. For $\alpha(\tau)$ = 11.63 W/(m^2·K), which holds at wind speeds ≤ 3 m/sec, the degree of freezing is 70% of the computed quantity performed for boundary conditions of the first kind. This difference is tracked well even for $\alpha(\tau)$ = 116.3 W/(m^2·K) (curves 3 and 4).

Approximate computations showed that the quantity of terms kept in the series should not be less than seven to achieve the requisite accuracy. The error in the computations grows abruptly with fewer series terms and the results are dubious.

On the whole, the developed method of solving the Stefan problem with arbitrary boundary conditions differs favorably from numerical methods assuming discretization in the coordinates and the time because of application of the analytic dependences (24), (25), and (29). None of the constraints inherent to the numerical method interferes in it.

NOTATION

Here $t_1(x, \tau)$, $t_2(x, \tau)$ are temperatures of the frozen and thawed phases; λ_1, λ_2; a_1, a_2, coefficient of thermal conductivity and diffusivity of the frozen and thawed phases; $t_m(\tau)$, $t_{surf}(\tau)$, environment and surface temperature; $q_{surf}(\tau)$, heat flux on the surface; $\alpha(\tau)$, heat transfer coefficient; $\xi(\tau)$, phase transition front coordinate; t_p, phase transition temperature; $\Theta_2(x)$, initial temperature of the thawed phase; τ, time; x, a coordinate; $y = (\xi(\tau)^2$; $\alpha_{ef}(\tau)$, effective heat transfer coefficient; $\lambda_{sn}(\tau)$, snow cover thickness; $\lambda_{sn}(\tau)$, snow heat-conduction coefficient. Subscripts 1 and 2 denote the frozen and thawed zones, respectively.

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