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CALCULATION OF TEMPERATURE FIELDS IN THE GROUND WITH WATER–ICE PHASE TRANSITIONS IN THE TEMPERATURE SPECTRUM

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An algorithm of integration of the nonlinear heat-conduction equation for a semi-bounded medium with a uniform initial distribution of temperature and its constant value on the surface in the case of nonlinear dependence of thermophysical characteristics on temperature is described. This algorithm can be used to test numerical grid methods of calculation of temperature fields in freezing and thawing of grounds. The procedure of correction of a step-by-step mechanism of temperature variation in numerical calculation in the zone of intense phase transitions by a grid method was suggested and tested.

The classical Stefan problem on determination of the temperature field in freezing of wet ground presupposes water–ice phase transitions at one point of the temperature range. However, experimental data on the phase state of water in grounds at a negative temperature show that for most soils and grounds that have in their composition clay and organogenic rocks freezing of the bulk of pore moisture occurs within the temperature range 0–10^{o}C. In this case, the temperature dependence of the amount of nonfrozen water is expressed by a nonlinear function that, on approaching 0^{o}C, asymptotically tends to ∞ [1].

Reduction of these problems to the Stefan-type problems with localization of phase transitions at a point, on the one hand, generates a number of problems typical of these problems and requires employment of special methods of their solution [2–4]; on the other hand, for soils and grounds where water–ice phase transitions occur in the temperature spectrum, the dependence of temperature on the coordinate in the frozen zone at the boundary with the thawed zone will be approximated insufficiently accurately. This will strongly complicate solution of problems on calculation of the processes of migration of moisture and water-soluble compounds in freezing rocks, since here it is necessary to know the exact value of the temperature gradient on the boundary between the zones. Then, solution of problems with phase transitions in the temperature spectrum by numerical grid methods is related to certain difficulties caused by a sharp change in the effective heat capacity in the zone of intense transitions. For example, even slight variations of temperature (of an order of 0.01^{o}C) can lead to a jump through the zone of main phase transitions, i.e., in transition through the point of the onset of freezing, the values of the effective heat capacity at the beginning and end of the temperature range $[T, T + \Delta T]$ can be much smaller than at its center. This results in great errors in the computation scheme. In order to estimate and improve the grid computation schemes we must have standard solutions of similar problems, which are obtained by analytical or other numerical methods. With this in mind, it is suggested to consider a method of integration of the nonlinear heat-conduction equation for a semi-bounded medium that admits a self-similar solution in numerical and analytical forms.

We consider a one-dimensional, heat-conduction equation with boundary conditions of the first kind in the homogeneous semi-bounded medium

$$\frac{\partial T(x,\tau)}{\partial \tau} C(T)\rho = \frac{\partial}{\partial x}\left[\lambda(T)\frac{\partial T(x,\tau)}{\partial x}\right], \quad T(x,0) = T_{\text{in}}, \quad T(0,\tau) = T_{\text{m}}, \quad T(\infty,\tau) = T_{\text{i}}. \tag{1}$$

We consider this equation in both freezing/thawing of wet ground and the mode when temperature preserves the sign, i.e., $T_{\text{in}}T_{\text{m}} \le 0$ and $T_{\text{in}}T_{\text{m}} > 0$.

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In order to solve Eq. (1) we use the method given in [5], where it is shown that, using the generalized variable $\xi = x/\sqrt{\tau}$, we can find a solution in the form of the nonlinear integral equation

$$T(\xi) = T_{\mathrm{m}} + A \int_0^{\xi} \frac{1}{\lambda(T)} \exp\left[- C(T) \int_0^{\zeta} \frac{\rho}{2\lambda(T)} \xi d\xi \right] d\zeta \,. \tag{2}$$

However, the given solution has an inaccuracy or a clerical error, which could be disregarded if it were not then given elsewhere [6]. The fact is that if heat capacity depends on temperature, the function $C(T)$ in the exponent must stay under the integral sign, which, as a result, leads to the following expression of the posed problem:

$$T(\xi) = T_{\mathrm{m}} + A \int_0^{\xi} \frac{1}{\lambda(T)} \exp\left[- \int_0^{\zeta} \frac{C(T)\rho}{2\lambda(T)} \xi d\xi \right] d\zeta \,,$$

$$A = \left\{ \int_0^{\infty} \frac{1}{\lambda(T)} \exp\left[- \int_0^{\zeta} \frac{C(T)\rho}{2\lambda(T)} \xi d\xi \right] d\zeta \right\}^{-1} . \tag{3}$$

To obtain a solution in a functional form, we must know the value of the integration factor A. Here we come across the problem of the recurrence of the formula: the factor A depends on the functions $\lambda(T)$ and $C(T)$ and on the initial temperature and the temperature on the ground surface.

Of certain difficulty in construction of the solution is the nonlinearity of the problem characteristics: the specific heat capacity is determined by a function that possesses a clearly pronounced nonlinearity caused by the dependence of the amount of nonfrozen water on temperature $W_{\mathrm{nfr}}(T)$. On approaching the point of the onset of freezing, the derivative of this function, which determines the effective heat capacity, increases sharply, thus changing by several orders.

The specific heat capacity and temperature of the onset of phase transitions T_{ph} for organogenic grounds can be calculated by the formulas

$$T_{\mathrm{ph}}(W) = T_0 - \left(\frac{a_1}{W - a_2} \right)^3 , \quad W_{\mathrm{nfr}}(T, W) = \begin{cases} a_1 (T_0 - T)^{-\frac{1}{3}} + a_2 \,, & T \le T_{\mathrm{ph}} \,; \\ W \,, & T > T_{\mathrm{ph}} \,, \end{cases}$$

$$C(T, W) = C_{\mathrm{a}} + \frac{\partial W_{\mathrm{nfr}}(T, W)}{\partial T} L \,. \tag{4}$$

By example, for peat the parameters of empirical approximation a_1 and a_2 have numerical values of 0.37 and 0.33 and the temperature of the onset of water freezing at a moisture content of 3 kg/kg is -0.002^{o}C. In this case, the effective heat capacity is $4 \cdot 10^8$ J/(kg·$^{\mathrm{o}}$C), which is more than five decimal orders higher than the additive heat capacity. This clearly pronounced nonlinearity imposes special conditions on the methods of integration of Eq. (3).

A search for solution of the heat-conduction equation is reduced to determination of the integration factor A at which temperature at the point $\xi \to \infty$ asymptotically tends to T_{in}. The principle of construction of the algorithm of determination of A is reduced to the following. The value of A is determined in the first approximation, for which we can use the formula

$$A = \frac{1}{\sqrt{\pi}} (T_{\mathrm{in}} - T_{\mathrm{m}}) \sqrt{\lambda_{\mathrm{im}} C_{\mathrm{im}} \rho} \,. \tag{5}$$

It is easy to check that at constant characteristics λ and C, having substituted the value of A from formula (5) into (3), we obtain the known solution of the heat-conduction equation expressed in terms of the function of the probability integral erf.

After determination of the first approximation of the value of A the step of integration with respect to ξ is chosen. In this case, allowing for a sharp change of thermophysical characteristics as a function of temperature in the vicinity of the point of phase transition T_{ph}, we determine the step $\Delta\xi$ by the equation

$$\Delta\xi = \frac{0.0001\sqrt{\lambda(T)}}{\sqrt{C(T)\rho}} . \tag{6}$$

The step over ξ ($\Delta\xi$) will be nonuniform during calculation; it depends on the problem characteristics. The factor of 0.0001 is chosen such that the step over T of an order of 10^{-3} (in the zones of smooth variation of the characteristics) and 10^{-5} (in the zones of their nonlinearity) could be provided in construction of the solution. This is necessary in order to obtain an authentic pattern of the distribution of T within the entire range of calculation.

We denote the expression under the exponent in formula (3) in terms of E, i.e.,

$$E = \int_0^{\zeta} \frac{C(T)\rho}{2\lambda(T)} \xi d\xi . \tag{7}$$

The integration procedure can be written as follows:

$$C = C(T + 0.5\Delta T) , \quad \lambda = \lambda(T + 0.5\Delta T) , \quad \Delta\xi = \frac{0.0001\sqrt{\lambda}}{\sqrt{C\rho}} , \quad \Delta E = \frac{C}{2\lambda}\rho(\xi + 0.5\Delta\xi)\Delta\xi , \quad E = E + 0.5\Delta E ,$$
$$\Delta T = A\frac{1}{\lambda}\exp(-E)\Delta\xi , \quad E = E + 0.5\Delta E , \quad T = T + \Delta T , \quad \xi = \xi + \Delta\xi . \tag{8}$$

In integration of Eq. (3) in the case of thawing of the ground that initially was in the frozen state there arises the problem with a jumpwise variation of the effective heat capacity from a comparatively low to a high value at the point of the onset of phase transitions T_{ph}. In this case, we come to a value of T_{ph} with a much larger step with respect to ξ as compared with its value immediately upon transition through this point. This results in the error of the solution obtained, since the coordinate that corresponds to T_{ph} is determined incorrectly.

To avoid this problem, we suggest the following procedure of correction of the step with respect to ξ, which allows one to determine the coordinate of T_{ph} with high accuracy. The essence of the procedure is as follows: as calculation approaches the point T_{ph}, we change the value of $\Delta\xi$ in order to pass through this point in one step and leave it with a minimum error; then we continue integration with account for the sharp variation of effective heat capacity due to water–ice phase transitions. In this case, the integration procedure appears as follows.

Values of the thermophysical characteristics C and λ are determined as functions of temperature at the center of the corresponding range and the integration step $\Delta\xi$ is found:

$$C = C(T + 0.5\Delta T) , \quad \lambda = \lambda(T + 0.5\Delta T) , \quad \Delta\xi = \frac{0.0001\sqrt{\lambda}}{\sqrt{C\rho}} .$$

Then values of the parameters S_1 and S_2 that characterize approach of temperature to the point of phase transitions are determined:

$$S_1 = T_{ph} - T , \quad S_2 = T_{ph} - T - \Delta T .$$

At a rather small value of the modulus of values of S_1 or S_2 a zero value is given to the corresponding parameter. Then, the sign of the product S_1S_2 is estimated and if it is less than zero then it is assumed that with variation of the current value of temperature by ΔT the jump through the point of phase transition T_{ph} took place. Therefore, in the cycle, variation of ΔT and $\Delta\xi$ is corrected by the formulas

$$\Delta T = T_{ph} - T , \quad \Delta\xi = \frac{\Delta T}{A\frac{1}{\lambda}\exp(-E + 0.5\Delta E) - \frac{\Delta T C\rho\xi}{4\lambda}} .$$

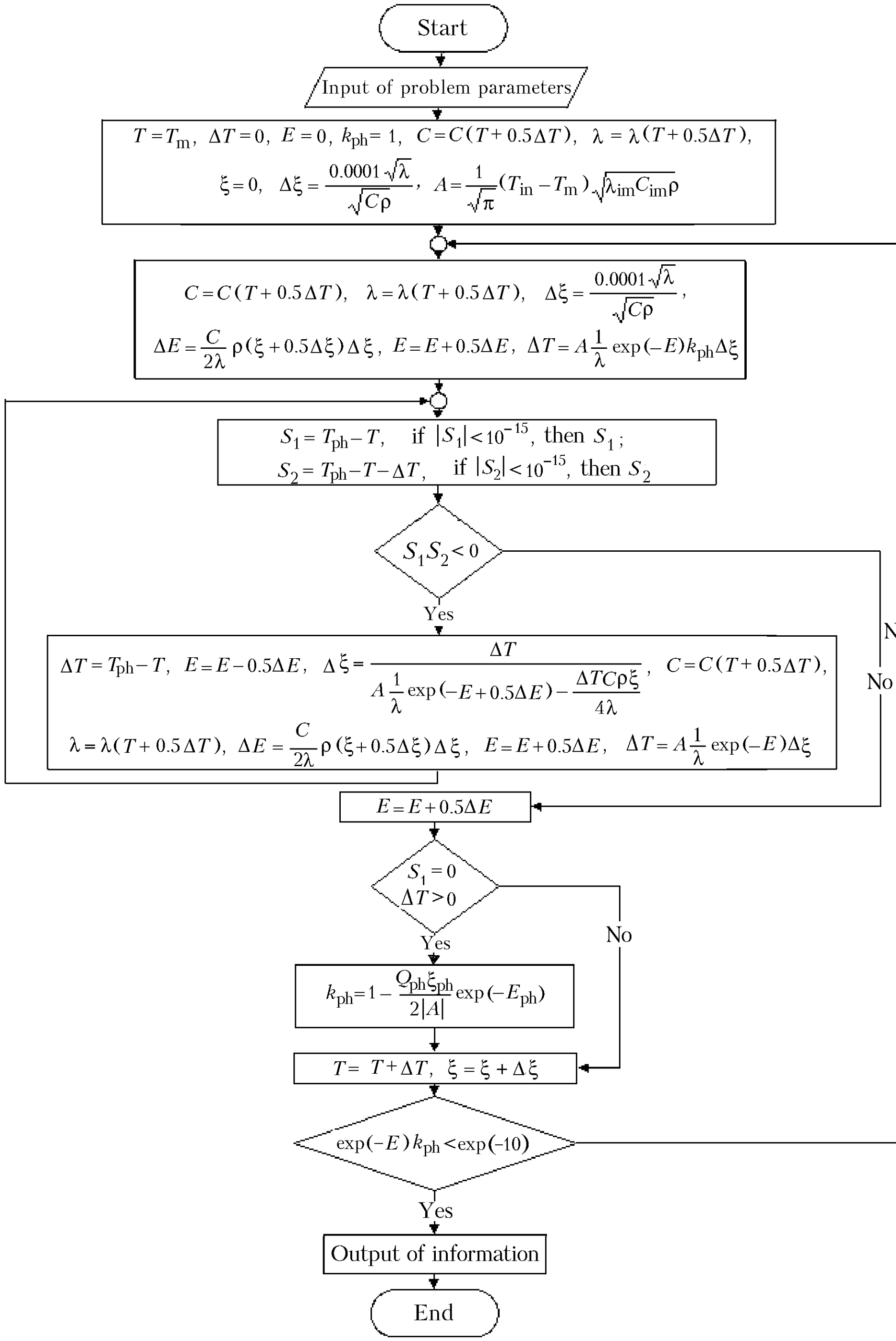

Fig. 1. Block-diagram of the algorithm of numerical integration of the non-linear heat-conduction equation.

Then, new values of ΔE, E, and ΔT are calculated by formulas similar to Eqs. (8) and we turn back to the start of the cycle. The cycle continues until the product S_1S_2 reaches an exact equality to zero, i.e., until new temperature values approach the value of T_{ph} with sufficient accuracy.

At a high moisture content in grounds when the temperature of the onset of phase transitions approaches 0^{o}C and the effective heat capacity tends to ∞, in the integration algorithm we can envisage the presence of the heat of phase transition Q_{ph} at the point T_{ph}. An analysis of the integral solution (3) showed that if the effective heat capacity tends to ∞ in a narrow temperature range and this temperature range tends to an infinitesimal quantity, the exponential factor exp ($-E$) which determines the temperature gradient changes jumpwise at the corresponding point. The calculations indicate that this variation can be expressed by introducing the coefficient k_{ph} by which the exponential factor is multiplied according to the formula

$$k_{ph} = 1 - \frac{Q_{ph}\xi_{ph}}{2\,|A|} \exp(E_{ph}) .$$

Exit from the integration procedure is determined by the condition under which $\exp(-E) < \exp(-10)$. In this case, the gradient T tends to zero and the temperature asymptotically reaches a constant value T_∞. If the thermophysical characteristics of the problem are uniform, assignment of the first approximation of A by formula (6) provides an accurate run into the value T_{in} and the first approximation of A is exact. When thermophysical characteristics depend on temperature, the initial approximation of A by formula (5) is not accurate and it must be corrected to provide $T_\infty \to T_{in}$. In further calculation, the integration procedure is supplemented with correction of the parameter A by the formula

$$A = A + \frac{1}{\sqrt{\pi}} (T_{in} - T_\infty) \sqrt{\lambda (T_\infty)\, C (T_\infty)\, \rho} .$$

After correction of A the integration cycle is repeated and the value of A is verified. The cycle of iterations is repeated until T_∞ reaches a value of T_{in} with sufficient accuracy. The block-diagram of the whole integration algorithm is given in Fig. 1.

Based on the suggested algorithm we developed a program of construction of the numerical solution of the problem. It allows one to construct the numerical dependence of T on ξ by the introduced characteristics. Initial data are assigned through the text file of a special format. The obtained result is also put into the file and is displayed in the form of the graph of the dependence $T(\xi)$. The developed algorithm makes it possible to obtain numerical solution of the linear heat-conduction equation virtually with any *a priori* specified accuracy.

The suggested algorithm allows one also to find an accurate analytical solution of the heat-conduction equation at piecewise-constant thermophysical characteristics within narrow temperature ranges and in the presence of the heat of phase transitions on the boundaries of these ranges. We consider such a problem. The entire temperature range from T_{in} to T_m is divided to n intervals. In each interval i, constant values of λ_i and C_i are specified. On the boundaries of some intervals at points T_i the heats of phase transitions Q_{phi} are specified. Introducing in a certain manner the value of thermophysical characteristics in each temperature interval, integrating Eq. (3) by the above-described algorithm, we can determine an accurate value of A. Using the latter, we write the corresponding solution of the heat-conduction equation in the analytical form as

$$T_1(\xi) - T_m = \frac{A\sqrt{\pi}}{\sqrt{\lambda_1 C_1 \rho}} \operatorname{erf}\left(\frac{\xi}{2\sqrt{a_1}}\right);$$

$$T_2(\xi) - T_1 = \frac{A\sqrt{\pi}}{\sqrt{\lambda_2 C_2 \rho}} \left[1 - \frac{Q_{ph1}\xi_1}{2\,|A|} \exp\left(\frac{\xi_1^2}{4a_1}\right)\right] \exp\left(\frac{\xi_1^2}{4a_2} - \frac{\xi_1^2}{4a_1}\right) \left[\operatorname{erf}\left(\frac{\xi}{2\sqrt{a_2}}\right) - \operatorname{erf}\left(\frac{\xi_1}{2\sqrt{a_2}}\right)\right];$$

$$E_i = \sum_{j=1}^{i} \frac{\xi_j^2 - \xi_{j-1}^2}{4a_j}\,; \quad k_{phi} = 1 - \frac{Q_{phi}\xi_i}{2\,|A|} \exp(E_i)\,; \tag{9}$$

$$T_i(\xi) - T_{i-1} = \frac{A\sqrt{\pi}}{\sqrt{\lambda_i C_i \rho}} \prod_{j=1}^{i} k_{phj} \exp\left(\frac{\xi_i^2}{4a_i} - E_i\right) \left[\operatorname{erf}\left(\frac{\xi}{2\sqrt{a_i}}\right) - \operatorname{erf}\left(\frac{\xi_{i-1}}{2\sqrt{a_i}}\right)\right].$$

Thus, we refined the technique of obtaining the solution of the nonlinear heat-conduction equation in numerical and analytical forms for a semi-bounded medium with uniform initial conditions, boundary conditions of the first

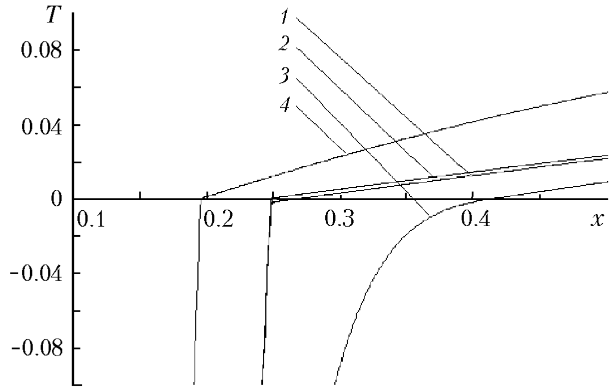

Fig. 2. Temperature distribution in the zone of intense water–ice phase transitions in different variants (1–4) of approximation of the dependence of the effective heat capacity on temperature in the freezing ground (T_m = –5^{o}C, T_{in} = +0.1^{o}C, τ = 10^6 sec).

kind, and for piecewise-constant characteristics within narrow temperature intervals and in the presence of the heat of phase transitions on the boundaries of these intervals. We should note that similar problems, which have the name of multifront Stefan-type problems, were in due time solved by V. G. Melamed [7], who wrote them in the form of a system of transcendental equations that express the Stefan condition on the boundaries between the zones. Specific realization of the obtained results is reduced to solution of the system of transcendental equations relative to the generalized coordinates of the points of phase transitions, which is a very complex problem. The solution obtained in our work in the form of (9) involves, in fact, one undetermined parameter A; the remaining parameters ξ_i, E_i, and k_{phi}, used in the solution, are successively calculated by the corresponding formulas beginning with the first temperature interval. The parameter A, as has been shown above, can be obtained from numerical solution of the nonlinear heat-conduction equation.

We should note that, in solving Stefan-type problems, in certain situations the method of approximation of the dependence of the effective heat capacity on temperature is of importance. Different methods of linearization of the dependence of the amount of nonfrozen water on temperature or localization of phase transitions at one point can lead to incorrect results, especially in calculation of the processes of freezing of grounds with an initial temperature close to 0^{o}C.

We now show by a specific example how much the results of calculation with different methods of approximation of the dependence of the effective heat capacity on temperature can differ. We consider the following problem. The initial temperature of the ground is +0.1^{o}C. A temperature of –5^{o}C immediately sets on the surface and remains constant all of the time. The moisture content of the ground W is 3.0 kg/kg and the density of the ground skeleton ρ_{sk} = 200 kg/m^3. The dependences of the amount of nonfrozen water and the effective heat capacity on temperature are described by formulas (4) with numerical values of the empirical coefficients a_1 = 0.37 and a_2 = 0.33. In solving this problem, we took four variants of approximation of the dependence of the effective heat capacity on temperature. In the first variant, we used a nonlinear dependence of the heat capacity on temperature according to formulas (3). In the second variant, up to temperature –0.01^{o}C we used an actual dependence of the amount of nonfrozen water on temperature, and then it was assumed that at the point T_{ph} = 0^{o}C water–ice phase transitions at a temperature of –0.01^{o}C take place. In the third variant, up to temperature –1.0^{o}C we used an actual dependence of the amount of nonfrozen water on temperature and then we took that within the temperature range from –1.0–0^{o}C this dependence is linear. The fourth variant corresponded to the classical Stefan problem, i.e., it was assumed that within the entire range of a negative temperature from –5 to 0^{o}C the amount of nonfrozen water changes from 0.47 to 1.0 kg/kg, the effective heat capacity remains constant, and the remaining amount of water is converted to ice at 0^{o}C. The results of the calculations of the indicated variants for time τ = 10^6 sec are given in Fig. 2.

It is seen from the data presented that the first and second variants virtually do not differ by the value of the freezing depth: in the first case it is 0.249 m and in the second — 0.248 m. At the same time, a thorough analysis of the results obtained showed that in the first variant, in the narrow zone on the freezing front the temperature gradient changes more smoothly and on the boundary between the thawed and frozen zones it is 4.62$^{\mathrm{o}}$C/m; in the second variant the same quantity is 10.85$^{\mathrm{o}}$C/m. Although this difference virtually does not affect the distribution of temperature, it can have an effect on calculation of the migration of moisture and water-soluble compounds in freezing grounds. As to the third and fourth variants, we can note that they strongly differ from the first variant by the value of the depth of freezing and the temperature gradient in the frozen zone on the front of freezing. Thus, for the third variant the depth of freezing is 0.409 m and the temperature gradient 0.108$^{\mathrm{o}}$C/m, and for the fourth variant the corresponding values are 0.195 m and 19.35$^{\mathrm{o}}$C/m.

As a result of the calculations we show that the methods of approximation of the dependence of the effective heat capacity on temperature can strongly affect the rate of freezing and the temperature distribution on the front of freezing. This effect is especially appreciable at the initial temperature of ground, close to 0$^{\mathrm{o}}$C. It follows from this fact that in calculation of the temperature fields in grounds one must use an actual nonlinear dependence of the amount of nonfrozen water on temperature. In this case, at relatively high moisture contents of grounds, when approaching 0$^{\mathrm{o}}$C within a very narrow range of temperatures the effective heat capacity reaches high values, it is possible to partially localize water–ice phase transitions at one point, admitting a jumpwise variation of the amount of nonfrozen water on the freezing front with the corresponding heat release Q_{ph}.

This technique of solving the nonlinear heat-conduction equation and the multifront Stefan-type problem can be used as a standard for testing numerical grid methods of solution of the problems of freezing (thawing) of soils and grounds. Using this technique one can estimate how accurately the tested method approximates the solution of the heat-conduction equation and choose optimum values of steps along the coordinate and time and also functions that approximate the dependence of thermophysical characteristics on temperature.

It should be noted that the suggested technique can be used for calculation of the processes of freezing and thawing of grounds with a uniform temperature distribution at the initial instant of time and constancy of temperature on the ground surface, i.e., in the cases where a self-similar solution is admitted. In the general case, in calculation of temperature fields in grounds with arbitrary initial and boundary conditions within the temperature range that includes intense phase transitions one must use numerical grid methods. However, in this case, a number of difficulties arise, which are caused by a sharp variation in the thermophysical characteristics. In particular, the calculation error can increase greatly due to a sharp change in the effective heat capacity and insufficiently accurate approximation of it in variation of temperature ΔT in a time step $\Delta\tau$ in the zone of intense phase transitions. Most often this can manifest itself in explicit computation schemes in calculation of the processes of heat and moisture transfer in grounds. To ensure conservativeness of these schemes, the computation algorithm must be additionally supplemented with the procedure of correction of temperature variation with account for conservation of heat balance.

The essence of the algorithms lies in verification of the fulfillment of heat balance in transition from the point of onset of freezing in a time step $\Delta\tau$. For this purpose, using the parameters S_1 and S_2 one compares the differences of temperature values relative to the point of onset of phase transition T_{ph} at the instants of time τ_i and $\tau_i + \Delta\tau$. If they appear to be of different signs, then variation of the enthalpy ΔH_i of an elementary volume at the grid node i in the time step $\Delta\tau$ is compared in absolute value with the value of the enthalpy H_0 which corresponds to the amount of heat necessary for variation of temperature to a value T_i at the time instant τ_i to the point of onset of phase transition T_{ph}. Depending on the ratio of these quantities and also on the sign of ΔH_i, ΔT_i is calculated in the time step $\Delta\tau$ or the iteration cycle of correction of temperature variation δT_i is introduced, which is based on the equations of heat balance for node i:

$$\Delta H_i = \left(\lambda \frac{T_{i-1} - T_i}{\Delta x} + \lambda \frac{T_{i+1} - T_i}{\Delta x}\right)\Delta\tau , \quad \delta T_i = \frac{(W(T_i + \Delta T_i) - W(T_i))\, L\rho\Delta x + C_{\mathrm{a}}\rho\Delta x\Delta T_i - \Delta H}{C_i\Delta x\rho} .$$

The block-diagram of the algorithm of calculation of temperature variation at node i is presented in Fig. 3. Fulfillment of all the procedures of the algorithm provides rather accurate satisfaction of the balance of thermal energy in the zone of intense phase transitions.

In testing this algorithm we used the standard solution of the nonlinear heat-conduction equation for a semi-bounded medium with uniform initial conditions and boundary conditions of the first kind, the procedure of development of which is described above. In this case, satisfactory agreement between the results obtained by the tested and standard methods is shown.

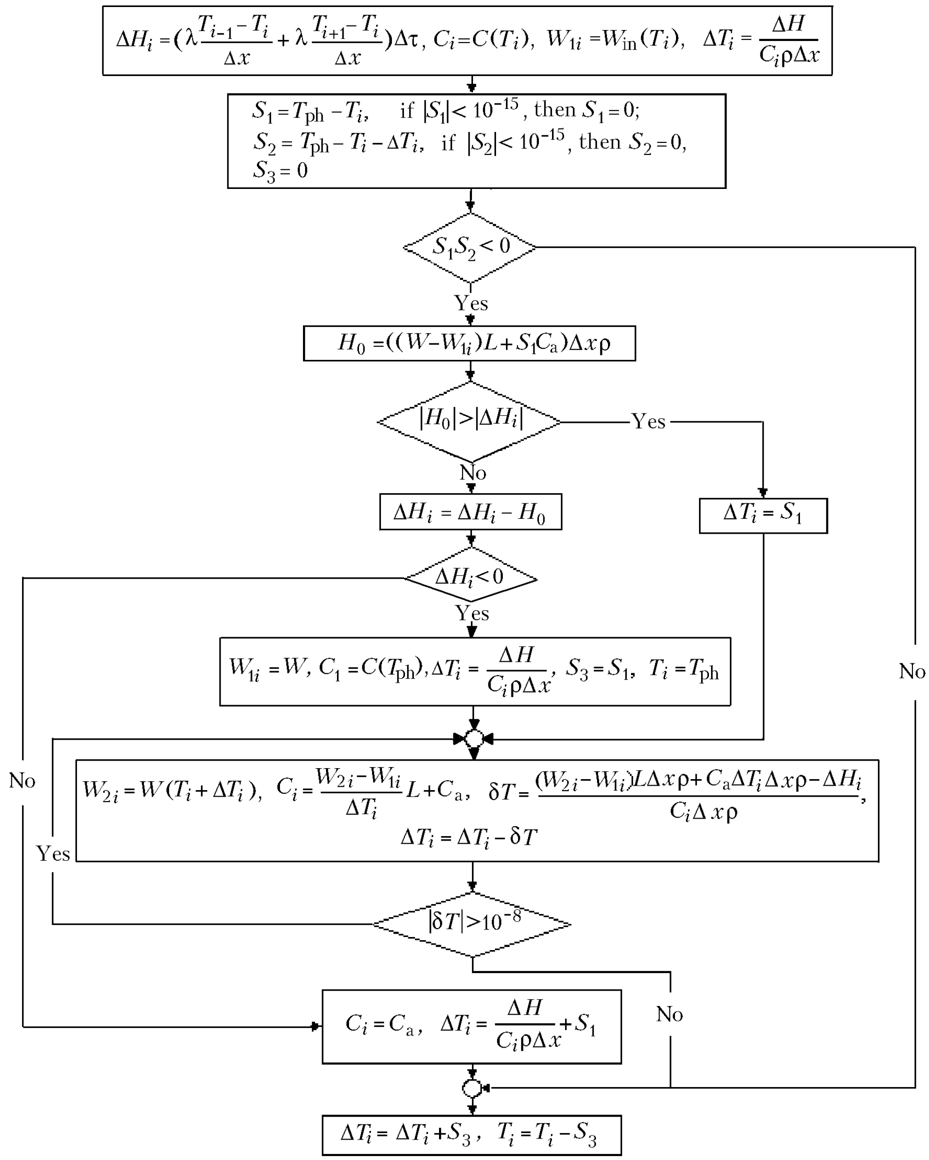

Fig. 3. Block-diagram of the algorithm of calculation of the temperature of phase transitions by a grid method.

In conclusion, we should note that calculation of two- and three-dimensional temperature fields in water–ice phase transitions is a rather complex problem, especially in localization of phase transitions at one temperature point. Therefore, it is rational to solve these problems by using the nonlinear dependence of the effective heat capacity on temperature according to a similar actual dependence of the amount of nonfrozen water within the entire temperature range under consideration. In such cases, numerical grid methods can be successfully used, employing the suggested algorithm of correction of the step-by-step variation of temperature on the basis of satisfaction of heat balance, since this algorithm has no principal difference for one- and multi-dimensional problems.

NOTATION

A, integration factor; a_1, empirical coefficient, $(^oC)^{1/3}$; a_2, empirical coefficient, kg/kg; *C*, specific heat capacity of the material, J/(kg·^{o}C); *E*, parameter of the exponential factor; *H*, enthalpy of an elementary volume, J/m^2; k_{ph}, coefficient of phase transition; *L*, heat of phase transition, J/kg; Q_{ph}, volumetric heat of phase transitions, J·m; S_1 and S_2, parameters of the computation scheme; *T*, temperature, ^{o}C; *W*, moisture content of the material, kg/kg; *x*, coordinate, m; λ, coefficient of thermal conductivity, W/(m·°C); ξ, generalized variable; ρ, material density, kg/m^3; τ, time, sec. Indices: m, medium; in, initial; nfr, nonfrozen; ph, phase transition; ∞, infinity; a, additive; sk, ground skeleton; im, integral-mean; *i*, index along the coordinate.

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