A PARAMETERS SELECTION CRITERION OF THE NUMERICAL REALISATION OF THE CONTINUOUS METHOD FOR THE STEFAN PROBLEMS

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This paper suggests a selection criterion of the continuous method version for a numerical solution of the Stefan problem which would allow to calculate the phase transition boundary position with a required accuracy for a long period of time and would enable generalisation to multidimensional problems. Despite a large number of works deal with the solution to the generalised Stefan problem by the continuous method, the choice of the smoothing interval value for numerical feasibility is not fully clear. A comparison of the calculation accuracy of the phase transition boundary position using different versions of the continuous method was carried out on an example of the well known one-dimensional plane two-phase Stefan problem which possesses an analytical solution. The dependence of the total error of the numerical calculation of the phase transition boundary position on the value of the smearing interval is determined from the comparison of numerical and analytical solutions. An analysis of the reason for increase of this error with time at any choice of a constant smoothing interval is given. A version of the continuous method with a variable interval of the delta function smoothing, in which the proposed criterion is carried out, is discussed. The position of the phase transition boundary calculated proposed version matches the analytical solution with a required accuracy over a long period of time.

Key words*: Stefan problem, glaciation, the continuous method version, numerical solutions, choice of the delta function smearing interval*

1. Introduction

For practical purposes, it is often more important to know the phase transition boundary that determines the thickness of the ice layer rather than knowing the temperature distribution. It is known that the position of the phase transition boundary can be calculated with acceptable accuracy using numerical methods that explicitly track the motion of this boundary [1], [2]. This is the front-tracking method, in which finite- difference schemes with adaptive or deformed grids are employed. However, front-tracking methods are difficult to apply in multidimensional problems [3]. As it is known, the transition to multidimensional problems is most simply realised in the continuous methods (enthalpy methods), in which the phase interface is not clearly distinguished and the problem is reduced to the solution of the generalised heat equation. The smoothing (smearing) of the specific heat capacity coefficient $c(T)$, the thermal conductivity coefficient $\lambda(T)$ and enthalpy $H(T)$ plays an essential role in this approach. The smoothing has no dependence on the dimension of a problem as one takes place with respect to the temperature T. These methods were almost simultaneously proposed and justified in 1965 by A. A. Samarskii and B. D. Moiseyenko [4] as well as B. M. Budak et al. [5]. In the 60s, S. L. Kamenomostskaya [6] introduced the concept of a generalised solution of the multidimensional Stefan problem. The heat conduction equations for different phases were treated as one equation for the enthalpy, which is a known function of temperature and has discontinuity of the first kind at the phase transition temperature. The existence and uniqueness theorems of the generalised solution of the multidimensional Stefan problem have been proved by O. L. Oleynik [7], S. L. Kamenomostskaya, and A. Fridman [8]. For one-dimensional problems, the enthalpy method was considered in [9]. Caldwell and Chan [10] have applied the enthalpy method to different types of geometries. However, there was no proof that the enthalpy formulation of the Stefan problem is equivalent to the classical one. In [11] the effect of the process of enthalpy smoothing was studied. Currently, there are many various realizations of the continuous method, for example [4], [5], [10–13]. Despite a large number of works that deal with the solution to the generalised Stefan problem by the continuous method, the choice of the smoothing interval value for numerical and computational feasibility is not fully clear. In this paper, the reason for impossibility to ensure required accuracy of the phase transition boundary calculation using the continuous method with a constant interval of smoothing the delta function for all moments of time is analyzed. We propose a selection criterion of the continuous method version for the numerical solution to the Stefan problem which would allow to correct this problem. The variant of the continuous method with a variable smearing interval of delta function, which provides the necessary accuracy of the calculation of the phase transition boundary for all moments of time, is presented.

It should be noted that the continuous method was created as a means of calculating mainly the phases temperature, rather than the phase transition boundary, which is not clearly distinguished in these methods.

2. Problem statement

To assess the effectiveness of the different versions of the continuous methods in the calculating of the phase boundary position a solution to the well known 1D two-phases Stefan problem for which the exact solution is known [3], [16] using these methods was considered.

It's known that all thermal and physical characteristics of growing sea ice depend on its salinity. The authors have previously proposed [15] the selection technique of a consistent set of thermo physical characteristics of growing sea ice. Based on these data, the following set of thermo physical characteristics and conditions was used in the calculations:

$$T_\infty = 272.15,\ T_* = 271.236,\ T_0 = 265.236,\ c_1 = 2150500,\ c_2 = 3995450, \qquad (1)$$

$$\lambda_1 = 2.0,\ \lambda_2 = 0.6,\ Q = 744584912.5.$$

Small values of the Stefan number are characteristic of the problems of glaciations in salt sea water. For parameter set (1) the Stefan number equals to 0.0173.

The one-dimensional plane two-phase Stefan problem is written as follows [16]:

$$c_1 \frac{\partial T_1}{\partial t} = \lambda_1 \frac{\partial^2 T_1}{\partial x^2},\ \ t > 0, \quad x \in \left(0, y(t)\right); \qquad (2)$$

$$t>0,\ x=0:\ T_1=T_0; \tag{3}$$

$$c_2\frac{\partial T_2}{\partial t}=\lambda_2\frac{\partial^2 T_2}{\partial x^2},\ t>0,\quad x\in\left(y(t),\infty\right); \tag{4}$$

$$t=0,\ x\in\left(0,\infty\right):\ T_2(x)=T_\infty; \tag{5}$$

$$t>0,\ x\to\infty:\ T_2=T_\infty; \tag{6}$$

$$t>0,\quad x=y(t):\ T_1=T_2=T_*; \tag{7}$$

$$\lambda_1\frac{\partial T_1}{\partial x}\bigg|_{y-0}-\lambda_2\frac{\partial T_2}{\partial x}\bigg|_{y+0}=Q\frac{dy}{dt}; \tag{8}$$

$$t=0:\ y=0. \tag{9}$$

The glaciation problems are characterised by the condition $T_0 < T_* < T_\infty$ under which the temperature of both ice and water is a monotonically increasing function in space and a monotonically decreasing function in time; $y(t)$ is a monotonically increasing function of time.

Problem (2)–(9) has a known analytical solution [16]:

$$T_1(x,t)=A_1+B_1\,\mathrm{erf}\left(\frac{x}{2a_2t^{1/2}}\right),\ T_2(x,t)\ =A_2+B_2\,\mathrm{erf}\left(\frac{x}{2a_2t^{1/2}}\right),\quad y(t)=\alpha t^{1/2}. \tag{10}$$

The constants a_k are equal to: $a_k=\left(\lambda_k/c_k\right)^{1/2}$, k = 1, 2; constants A_1, A_2, B_1, and B_2 in a known manner are expressed through the parameters of the problem (2)–(9) and the value of α, which is calculated by the transcendental equation given in [16], and depends on all parameters of the problem, namely T_0, c_1, c_2, λ_1, λ_2, Q, T_*, and T_∞.

Let us consider the numerical solution to the Stefan problem (2)–(9) by the continuous method proposed in [4]. For constant thermophysical coefficients c_1, c_2, λ_1, and λ_2 the solution to the problem in the region $x \in (0, \infty)$ with boundary conditions (3), (6), and initial condition (5) is reduced to the solution of the generalised heat equation

$$\left\{c(T)+Q\delta(T-T_*)\right\}\frac{\partial T}{\partial t}=\frac{\partial}{\partial x}\left(\lambda(T)\frac{\partial T}{\partial x}\right), \tag{11}$$

$$c(T)=\begin{cases}c_1 & \text{at}\quad T<T_*,\\ c_2 & \text{at}\quad T>T_*,\end{cases}\qquad \lambda(T)=\begin{cases}\lambda_1 & \text{at}\quad T<T_*,\\ \lambda_2 & \text{at}\quad T>T_*,\end{cases} \tag{12}$$

where $\delta(\xi)$ is a Dirac delta function. The solution $T(x,t)$ to the generalised equation (11) under conditions (12), satisfies the heat equations (2) and (4) outside the phase transition boundary. At the boundary of the phase transition, the heat flux and enthalpy are discontinuous functions therefore the fulfillment of the Stefan condition (8) is proven in the integral sense [4]. The proof is based on the properties of the delta function and on the condition of the movable boundary $x=y(t)$ of the phase transition.

In the transition to the numerical solution of Eq. (11), the Dirac delta function is replaced by a delta-shaped (smeared) delta function with the value of the smearing half-interval Δ. If in each of the phases the coefficients c_1 and c_2 are considered constant, the simplest interpolation of the jump in enthalpy at the transition phase boundary is linear, which corresponds to the following representation of the effective heat capacity $\{c(T)+Q\delta(T-T_*)\}=c(T,\Delta)$:

$$c(T,\Delta)=\begin{cases} c_1, & T<T_*-\Delta, \\ \dfrac{c_1+c_2}{2}+\dfrac{Q}{2\Delta}, & T_*-\Delta<T<T_*+\Delta, \\ c_2, & T>T_*+\Delta. \end{cases} \tag{13}$$

At the same temperature interval the effective thermal conductivity is assumed $\lambda(T)=\lambda(T,\Delta)$,

$$\lambda(T,\Delta)=\begin{cases} \lambda_1, & T<T_*-\Delta, \\ \dfrac{\lambda_1+\lambda_2}{2}, & T_*-\Delta<T<T_*+\Delta, \\ \lambda_2, & T>T_*+\Delta. \end{cases} \tag{14}$$

The solution of Eq. (11) is replaced by the solution of the equation with smoothed coefficients

$$c(T,\Delta)\frac{\partial T}{\partial t}=\frac{\partial}{\partial x}\left(\lambda(T,\Delta)\frac{\partial T}{\partial x}\right) \tag{15}$$

With appropriate initial and boundary conditions for the temperature $T(x,t,\Delta)$. The matter of convergence of the solution of equation (15) to the solution of equation (11) at $\Delta\to 0$ is considered in [7].

3. Numerical solution

Eq. (15) for the set of parameters (1) was solved by the continuous method using an implicit scheme, in which the smoothed coefficients $c(T,\Delta)$ and $\lambda(T,\Delta)$ were calculated at the previous time step by formulas (13) and (14). The continuous method proposed in [4], does not answer the question of choosing the value of the interval Δ of the delta function smearing. Despite a lot of work on the study of the solution to the generalised Stefan problem by the continuous method, the choice of the interval Δ is unclear.

In this paper, at the constant values of dimensionless steps h and τ (steps in space and time respectively) as a result of the computational experiment has been found the value Δ, at which the sum of deviations of the ice layer thicknesses, calculated numerically from values, found from analytical solution of the problem is the minimum on the studied time interval.

The first conclusion to which the calculations led was as follows: the numerical value of the ice boundary y^n is closest to its analytical value $y(t^n)$ for the time interval $(0,t_{end})$, t_{end} = 23.22 [h], if it is required that the temperature interval from $T_*-\Delta$ to $T_*+\Delta$ for any time moment t^n from the interval $(0,t_{end})$ contains no more than two nodes x. To fulfill this requirement for the chosen h and τ was found the range of permissible values Δ, for which in each time moment t^n there exists a node i_n such that the following conditions are carried out

$$T^n_{i_n-1}<T_*-\Delta,\ T^n_{i_n+1}<T_*+\Delta,\ T^n_{i_n+1}-T^n_{i_n-1}>2\Delta,\ \forall t^n\in(0,t_{end}). \tag{16}$$

From these conditions it follows that $x_{i_n-1} < y^n < x_{i_n+1}$. The thickness of the ice layer was assumed to be $y^n = x_{i_n}$. If we do not require conditions (16) and allow three or more nodes in *x* to fall within the specified temperature range, the position of the ice boundary y^n is determined by the found temperature array as the coordinate x_i of the node in which the temperature T_i^n is closest to the phase transition temperature T_*. However, under this approach, all other things being equal, the error in the calculation of y^n is significantly greater than in the calculation using the conditions (16).

Among all the permissible values of the interval Δ, satisfying conditions (16) for a given *h* and τ, a value was chosen for which the sum of deviations y^n from the analytical solution $y(t^n)$ is minimal for a given time interval. Discussion of the results of the choice of Δ, as well as examples of calculations are given in the following sections.

The problem was solved under the following conditions: the initial thickness y_0 of the ice layer (a multiple of step *x*) was given, using this value y_0 the initial time t_0 from the analytical solution (10) and the initial temperature distribution $T_1^{(0)}(x,t_0)$ in the ice layer were calculated. In addition, according to the analytical solution (10), the initial temperature distribution $T_2^{(0)}(x,t_0)$ in the water layer of length $l(t_0)$ was found.

The smoothed Eq. (15) under the selected initial conditions was solved numerically by the algorithm based on the fulfillment of the requirements (16). For different values of the interval Δ the temperatures which found using the numerically calculated values $y^n(\Delta)$ of ice layer thicknesses at the time moments t^n were compared with the exact values of $y(t^n) = \alpha(t^n)^{1/2}$ (10) under the same initial conditions. Examples of comparisons are presented in tab. 2 for a set of parameters (1) at y_0 = =0.5 [cm], $t_0 = 13.2$ [min], values of dimensionless steps *h* = 0.1, τ = 1, and for the specified values of the temperature interval Δ. For the set of parameters (1) the value of α was 0.0001777 [m/s$^{1/2}$]. Tab.2 shows the dimensional values of $y(t^n) = \alpha(t^n)^{1/2}$ and the values of deviations $\delta_m = y(t^n) - y^n(\Delta_m)$, *m* = 1, 2, 3 for different moments of time measured from *t* = 0.

The interval $(0, t_{end})$ was used to calculate the total error $S(\Delta)$ defined as $S(\Delta) = \sum_{n=1}^{N} \left| y(t^n) - y^n(\Delta) \right|$, where *N* is the number of time steps. In tab. 1 the dependence of the total error $S(\Delta)$ [cm] from Δ [K] in the time interval $(0, t_{end})$ at t_{end} =23.22 [h] is presented.

Table 1. The dependence of the total error *S* from Δ

$\Delta \cdot 10^3$	5.7	5.6	5.5	5.4	5.3	5.0	4.0
$S(\Delta)$	396.8	392.4	390.5	389.7	391.9	415.9	741.2

It follows from tab. 1 that for the accepted parameters of the problem the total error $S(\Delta)$ in the numerical calculation of the ice layer thickness $y^n(\Delta)$ is minimal at Δ = 0.0054. We give the exact values of the ice layer thickness $y(t^n)$ and the deviation δ_m [cm] at different values of Δ.

Table 2. The values of $y(t^n)$ and deviations δ_m, *m* = 1, 2, 3.

t	0.55	1.22	4.82	9.42	11.72	16.32	18.62	23.22
$y(t^n)$	0.793	1.177	2.340	3.272	3.649	4.306	4.602	5.137
$\delta_1\ (\Delta_1 = 0.006)$	0.193	0.377	0.440	0.172	0.049	-0.193	-0.400	-0.663
$\delta_2\ (\Delta_2 = 0.0054)$	0.193	0.377	0.440	0.372	0.249	0.006	-0.200	-0.463
$\delta_3\ (\Delta_1 = 0.005)$	0.193	0.377	0.540	0.372	0.349	0.106	0.000	-0.263

The performed calculations, some of which are presented in tab. 2, led to the conclusion that it is not possible to calculate the thickness of the ice layer for the entire time interval with a required accuracy for the specified version of the continuous method with constants h, τ and Δ. The biggest drawback for large time intervals is the error in the calculation of $y^n(\Delta)$ that increases over time. This takes place in the settlements for any permissible value of Δ. This state of affairs was also noted in a number of works such as [17].

This conclusion is valid for the quadratic approximation of the delta function in the interval $T_* - \Delta < T < T_* + \Delta$, and for the calculation of the smoothed coefficients $c(T,\Delta)$ and $\lambda(T,\Delta)$ at the calculated time step using the iterative method of solving a nonlinear system of difference equations. Earlier calculations of surface glaciation in seawater showed that the value of Δ when using the continuous method with a constant interval Δ has a greater influence on the accuracy of coincidence with known solutions than the choice of the interpolation polynomial. Of course, it is possible to achieve a local improvement in the accuracy of the calculation by choosing a higher order polynomial in the smoothing of the delta function and the coefficients of heat capacity and thermal conductivity. However and in this case it is not possible to avoid the increase over time of the error in the calculation of $y^n(\Delta)$ at any permissible constant Δ.

4. Analysis of the cause of the increasing error in the calculation of the position of the phase transition boundary at the constant h, τ, and Δ

We estimate the error with which the Stefan condition (8) is satisfied in the numerical solution to the smoothed Eq. (15). We write the integral equation of the balance of internal energy ε of the resting medium in the absence of sources (sinks) and external forces. The rate of change in time of the internal energy of the medium density ρ in region *G* is equal to, in this case, the total heat flux through a closed surface S_G of region *G*. Assuming that the heat flux $\vec{j}$ is determined by the Fourier law: $\vec{j} = -\lambda\ \mathrm{grad}T$, we come to the integral equality

$$\int_G \frac{\partial \rho\varepsilon}{\partial t} dv = \iint_{S_G} \lambda \ \mathrm{grad} T \cdot \vec{n} ds, \tag{17}$$

where $\vec{n}$ is the external normal to the surface of region G.

Under the assumptions made, the pressure p does not depend on time, therefore in Eq. (20) we can move from the volume density ρ, ε of internal energy to the volume density ρu of the enthalpy of the medium:

$$\rho\varepsilon = \rho u - p \ \rightarrow \ \frac{\partial \rho\varepsilon}{\partial t} = \frac{\partial \rho u}{\partial t}. \tag{18}$$

Let us denote the volume density ρu of the enthalpy by H. In the one-dimensional problem the integral equation (17) with (18) for the interval [$x_{i_n} - h, x_{i_n} + h$] is written as:

$$\int_{x_{i_n}-h}^{x_{i_n}+h} \frac{\partial H}{\partial t} dx = -\left(\lambda_1 \frac{\partial T}{\partial x}\bigg|_{x_{i_n}-h} - \lambda_2 \frac{\partial T}{\partial x}\bigg|_{x_{i_n}+h} \right). \tag{19}$$

When crossing the ice-water boundary, the enthalpy H has discontinuity of the first kind, the magnitude of the jump of the enthalpy is equal to Q. With constant heat capacity coefficients and constant densities of ice and water, the enthalpy H depends on the temperature T as follows:

$$H(T) = \begin{cases} c_1 \mathrm{T} & \text{at} \quad T < T_*, \\ c_1 \mathrm{T}_* + Q + c_2 (T - T_*) & \text{at} \quad T > T_*. \end{cases} \tag{20}$$

In the paper [18] for the three-dimensional version of the two-phase Stefan problem, the fulfillment of the Stefan condition (8) in the integral sense in the enthalpy notation of the generalised equation (11) is proven. We turn to the smoothed functions of enthalpy $H(T,\Delta)$ and temperature $T(x,t,\Delta)$. It can be shown that in the case of linear interpolation of the enthalpy jump (20) the expression for the derivative $\partial H/\partial t$ from the smoothed enthalpy is written as

$$\frac{\partial H}{\partial t} = \frac{dH}{dT}\frac{\partial T}{\partial t} = \left(\frac{c_1 + c_2}{2} + \frac{Q}{2\Delta} \right) \frac{\partial T}{\partial t}, \tag{21}$$

the constant value of Δ in Eq. (22) is expressed by c_1, c_2, and T_*. In problems of glaciation of surfaces in sea water, typical value of $Q/(2\Delta)$ is at least three orders of magnitude greater than the values of c_1 and c_2 for any Δ, satisfying the inequality $\Delta < 1$. Consequently, the terms $(c_1 + c_2)/2$ in Eq. (21) can be neglected in comparison with the $Q/(2\Delta)$ term. Thus, the equality (19) for smoothed functions $H(T,\Delta)$ and $T(x,t,\Delta)$ can be written as an approximate equality

$$\frac{Q}{2\Delta} \int_{x_{i_n}-h}^{x_{i_n}+h} \frac{\partial H}{\partial t} dx \approx -\left(\lambda_1 \frac{\partial T}{\partial x}\bigg|_{x_{i_n}-h} - \lambda_2 \frac{\partial T}{\partial x}\bigg|_{x_{i_n}+h} \right). \tag{22}$$

The derivative $\partial T/\partial t$ from the smoothed function $T(x,t,\Delta)$ on the interval $[\,x_{i_n}-h, x_{i_n}+h\,]$ is continuous and hence the integral in the left part of Eq. (22) is equal to $\int_{x_{i_n}-h}^{x_{i_n}+h}\frac{\partial T}{\partial t}dx \approx \left.\frac{\partial T}{\partial t}\right|_{x_*} 2h,$ $x_* \in [\,x_{i_n}-h, x_{i_n}+h\,]$. For $h \to 0$ from condition (16) it follows that: $x_* \to x_{i_n}$, $x_{i_n} \to y^n$ this allows us to write the approximate equality $\int_{x_{i_n}-h}^{x_{i_n}+h}\frac{\partial T}{\partial t}dx \approx \left.\frac{\partial T}{\partial t}\right|_{y^n} 2h.$ For the smoothed temperature, the condition (7) must be satisfied: $T(y^n,t^n,\Delta)=T_* =$ const $\forall t^n>0$, from which the approximate equation at the moving boundary of the phase transition follows: $\left.\frac{\partial T}{\partial t}\right|_{y^n} \approx -\left.\frac{dy}{dt}\right|_{t^n}\left.\frac{\partial T}{\partial x}\right|_{y^n}$.

Taking into account Eq. (22) for the time moment t^n we come to the next approximate analogue of the Stefan condition (8):

$$\lambda_1 \left.\frac{\partial T}{\partial x}\right|_{y^n-h} - \lambda_2 \left.\frac{\partial T}{\partial x}\right|_{y^n+h} \approx Q\left.\frac{dy}{dt}\right|_{t^n}\left(\frac{1}{\Delta}\left.\frac{\partial T}{\partial x}\right|_{y^n} h\right). \tag{23}$$

Let us find out the spatial interval h_Δ which corresponds to the temperature smoothing and enthalpy interval Δ. The interval h_Δ is determined by $\forall t^n>0$: $T(y^n,t^n,\Delta)=T_*$, $T(y^n+h_\Delta,t^n,\Delta)=T_*+\Delta$, $T(y^n-h_\Delta,t^n,\Delta)=T_*-\Delta$. A Taylor series expansion of the function $T(x,t,\Delta)$ about $x=y^n$ leads to:

$$T(y^n+h_\Delta,t^n,\Delta) \approx T(y^n,t^n,\Delta)+\left.\frac{\partial T}{\partial x}\right|_{y^n} h_\Delta \to T_*+\Delta \approx T_*+\left.\frac{\partial T}{\partial x}\right|_{y^n} h_\Delta \to \quad h_\Delta \approx \Delta\Big/\left(\left.\frac{\partial T}{\partial x}\right|_{y^n}\right). \tag{24}$$

4.1. A criteria of the Stefan condition fulfillment in the numerical solution of the smoothed heat equation for all moments of time

We denote the factor multiplying $Q\left.\frac{dy}{dt}\right|_{t^n}$ in the right part of equation (23) by K:

$$K=\left(\frac{1}{\Delta}\left.\frac{\partial T}{\partial x}\right|_{y^n} h\right) \approx \frac{h}{h_\Delta}. \tag{25}$$

As follows from Eq. (23), the Stefan condition (8) when $h\to 0$ in the numerical solution of the smoothed Eq. (15) holds for all points in time, if the following condition is satisfied

$$K=h/h_\Delta \approx 1 \qquad \forall t^n>0 \tag{26}$$

The analysis in the framework of the accepted assumptions allow us to explain why in the considered unsteady Stefan problem at large times the error in the calculation of y^n by this continuous method can not be eliminated for any value of *the constant interval* Δ for *the constants* h and τ. The fact is that the value of h_Δ, as follows from Eq. (24), is not constant. Under condition (10), the derivative $\left.\frac{\partial T}{\partial x}\right|_{y^n}$ decreases with time and at the constants h, τ, and Δ the value of h_Δ increases and the value of K decreases. The decrease in the time of the factor K in the approximate equality (23) indicates a distortion of the Stefan condition in the numerical solution of the smoothed Eq. (15) by this method. By selecting Δ, it is possible to achieve the condition $K \approx 1$ at some point in time, but with increasing time the condition (26) will inevitably be violated. In fact, this leads to the following: the numerical calculation of y^n occurs with an increasingly distorted Stefan condition, with a decrease in K it leads to an overestimation of the numerically calculated value of y^n in this problem. Indeed, one can show that when the multiplier in front of the derivative is reduced in the Stefan condition (8), the rate of glaciation and the thickness of the layer of ice increase. For example, for a set of parameters (1) with a decrease in Q by 2 times, the value of α (and with it the value of $y(t)=\alpha t^{1/2}$) increases by 1.404 times. This situation is demonstrated by the data in tab. 2.

Note that, it is possible to ensure the fulfillment of condition (26) and at a constant Δ due to the corresponding choice of variable space step.

4.2. A variant of the continuous method for calculating the position of the phase transition boundary for a long time interval with acceptable accuracy

Various variants of the continuous method allowing generalization to the multidimensional Stefan problems were considered. The greatest interest was aroused by the version published in a series of works by V. I. Vasil'eva et. al.(e.g. [19]). Within the frames of this method it possible to ensure the fulfillment of condition (26) at all time interval, and as shown in [19], the method is generalised to multidimensional problems with phase transitions.

Let us use a version of continuous method, in which condition (26) is met, to solve the test problem (1)–(7) with non-zero initial conditions. The proposed variant of the continuous method differs from the version of work [19] only by approximating the effective heat capacity coefficient. The finite-difference analog of the problem for internal nodes of the space-time grid is constructed as follows. Discontinuous coefficients of heat capacity, thermal conductivity, and the Dirac delta function are smoothed by temperature $T(x,t)$ only in the intervals containing the phase transition boundary, i.e. in the intervals where the inequalities $T_i^n \le T_* \le T_{i+1}^n$ are satisfied. For all other intervals, the discrete analog of Eq. (15) is a three-point difference equation approximating the usual heat equation with constant coefficients in the corresponding phase.

The approximation of the effective heat capacity and effective heat conductivity coefficients is written as follows:

$$\theta_n = \frac{T_* - T_i^n}{T_{i+1}^n - T_i^n}, \quad T_i^n \le T_* \le T_{i+1}^n \tag{27}$$

$$c(T_i^n, T_{i+1}^n) = \begin{cases} c_1, & T_i^n < T_*, \ T_{i+1}^n < T_*, \\ \theta_n c_1 + (1-\theta_n)c_2 + \dfrac{Q}{T_{i+1}^n - T_i^n}, & T_i^n < T_* < T_{i+1}^n, \\ c_2, & T_i^n > T_*, \ T_{i+1}^n > T_*. \end{cases} \tag{28}$$

$$\lambda(T_i^n, T_{i+1}^n) = \begin{cases} \lambda_1, & T_i^n < T_*, \ T_{i+1}^n < T_*, \\ \theta_n \lambda_1 + (1-\theta_n)\lambda_2, & T_i^n < T_* < T_{i+1}^n, \\ \lambda_2, & T_i^n > T_*, \ T_{i+1}^n > T_*. \end{cases} \tag{29}$$

$$y^n = (1+\theta^n)h.$$

The smoothed Eq. (15) with approximations (28), (29) was solved numerically by an implicit scheme. On each time layer the nonlinear system of difference equations was solved by fixed point iteration method. On each iteration the system of linear equations was solved by the tridiagonal matrix algorithm. The ending condition of the iterative process is when the following inequality is satisfied: $\max\limits_i \left| T_i^{s+1} - T_i^s \right| < \varepsilon_*$, here ε_* is the required temperature calculation accuracy, s is the iteration number. For $\varepsilon_* = 0.001$ [K], the number of iterations in the calculations did not exceed 3. Other parameters, such as initial data, set (1), and the length of thermal influence were the same as for the solution of this problem with constant Δ . It is easy to see that the factor K (25), introduced above, remains close to unity for all moments of time when approximating (28). This gave reason to expect that the deviations $\delta = y(t^n) - y^n$ of the values y^n , calculated by this variant of the continuous method from the values $y(t^n)$, found from the analytical solution of the problem will be small for all moments of time. The calculations confirmed the expectation. Note that this method requires a preliminary analysis of the choice of steps τ and h, it is necessary that in one step in time the boundary of the phase transition either remained in the same spatial interval, or passed into the adjacent interval. In tab. 3 the calculated values of deviations $\delta = y(t^n) - y^n$ for different moments of time are presented. Dimensionless steps h and τ were the same as in the calculation of the data in tab. 2.

Table 3. The values of deviations δ

t	0.55	1.22	4.82	9.42	11.72	16.32	18.62	23.22
δ	-0.031	-0.047	-0.053	-0.049	-0.048	-0.046	-0.042	-0.038

In fig. 1, we present a comparison of the time dependences of the deviations δ^n calculated by the proposed method and the continuous method at the constant Δ ($\Delta = 0.0054$).

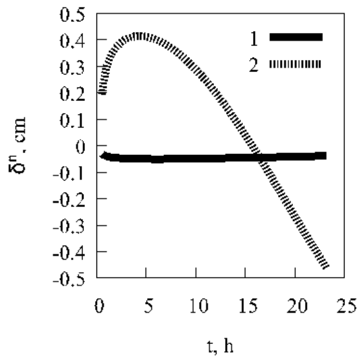

Figure 1. The time dependencies of the deviations δ^n : 1 — the proposed method; 2 — the continuous method at the constant Δ ($\Delta = 0.0054$).

Fig. 1 demonstrates the advantage of the method in which condition (26) is satisfied to calculate the position of the phase transition boundary. For the same parameters of the problem and the same values of h and τ , for the same time interval as in the calculation by the continuous method with a constant Δ , the total error S in the calculation by the method based on approximations (28) and (29), was the value: $S = \sum_{n=1}^{N} \left| y(t^n - y^n) \right| = 63.64$ which is almost an order of magnitude less than the minimum total error $S(\Delta = 0.0054) = 389.7$ of the solution of this problem by the continuous method with a constant Δ . It is particularly important in the calculation of long-term processes of glaciation in seawater that the continuous calculation method, based on approximations (28) and (29), does not lead to an increase in the error of calculation of the glaciation boundary over time.

Finally, as stated above, the difference of the proposed method from the method of work [19] consists in the approximation of the effective heat capacity coefficient. More specifically, in [19] the factor θ_n (27) in the summand $Q / (T_{i+1}^n - T_i^n)$ included in Eq. (28) was added. This summand in [19] was written as $Q\theta_n / (T_{i+1}^n - T_i^n)$. It is not difficult to see that using the approximation with this summand violates condition (26). Perhaps this has led to the substantial total error which surpassed by over 14 times the value S = 63.64.

The study of the convergence of the proposed version of the continuous method with the smoothing interval Δ, proportional to the temperature gradient is beyond the scope of this paper. Note that the solution of the classical Stefan problem (2)−(9), as is known, exists only and coincides with the generalised solution. As shown in this paper, the numerical solution of the generalised problem for the proposed version of the continuous method coincides with the classical solution with an accuracy of tenths of a percent over the entire time interval. This indicates that, at least for the solved Stefan problem, the proposed version of the continuous method converges and one converges to the classical solution of the problem.

5. Results and Conclusions

The paper discusses various versions of the continuous method for solving the Stefan problem. Using the example of a test problem that has an exact analytical solution, it is shown that the error in the numerical calculation of the phase transition boundary depends on the value of the smearing parameter of the delta function in the generalized heat equation. The computational experiments have led to the conclusion that it is impossible to ensure the required accuracy of calculating the phase transition boundary by the continuous method counting at a constant interval of smoothing the delta function and with constant steps in time and space for all time moments.

A criteria is proposed, the fulfillment of which provides the necessary accuracy of the calculation of the phase transition boundary for all moments of time in the numerical solution of the Stefan problem by the continuous method.

A variant of the continuous method with a variable smearing interval of delta function, in which the stated criteria is satisfied, is presented. The possibility to calculate using this method the position of the phase transition boundary during a long period of time with the necessary accuracy is demonstrated. It is shown that the calculation of the phase transition boundary by the proposed continuous method during the first day is an order of magnitude more accurate than the best variant of the continuous method at a constant Δ. It is significant that the accuracy of calculating the phase transition boundary by the proposed method practically does not change with time.

Nomenclature

c_k	coefficient of specific volumetric heat capacity of the *k*-th phase, [J m^{-3} K^{-1}],
H	enthalpy, [J m^{-3}],
λ_k	thermal conductivity coefficient of the k-th phase, [W m^{-1} K^{-1}],
Q	specific (per unit volume) heat of phase transition, [J m^{-3}],
S	total error, [cm],
T_∞	temperature of sea water, [K],
T_*	phase transition temperature, [K],
T_0	temperature on a given surface, [K],
$T_k(x,t)$	temperature of the *k*-th phase, [K],
y	coordinate of the phase transition boundary (ice layer thickness), [cm],
Δ	value of the smoothing interval, [K],
ρ	medium density, [kg/m^3],
ε	internal energy, [J/kg].

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