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IDENTIFICATION OF THE BOUNDARY MODE IN ONE THERMAL PROBLEM BASED ON THE SINGLE-PHASE STEFAN MODEL

Abstract. The process of melting a one-dimensional block of ice by heating it from the left border is considered. A one-dimensional Stefan model is proposed for the mathematical description of the melting process. It describes the temperature change in the resulting melt zone with a movable boundary. Within the framework of this model, the task is to identify the heating mode on the border of the block, which ensures the movement of the movable boundary of the melt zone according to a predetermined law. The posed inverse problem for the single-phase Stefan model belongs to the class of inverse boundary-value problems. With the use of the method of front straightening, the problem area with a movable boundary is transformed into a domain with fixed boundaries. A discrete analog of the inverse problem for each discrete value of the time variable splits into two independent second-order difference problems, for which the absolutely stable Thomas method is used, and a linear equation with respect to the approximate value of the heating temperature at the left boundary of the block. Numerical experiments were carried out on the basis of the proposed computational algorithm.

Keywords: heat transfer with phase transformation, ice melting process, movable phase interface, front rectification method, boundary inverse problem, difference method.

INTRODUCTION

It is known that the study of heat transfer processes taking into account phase transformations is an important task in many fields of science and technology. Examples of physical phenomena and processes with phase transformations are: the process of melting ice with an unknown time-varying boundary between water and ice, the process of melting a solid with an unknown boundary between solid and liquid phases, the process of concentration redistribution during mutual diffusion in a metal alloy with movable phase boundaries, etc. Such processes occur in a number of modern metallurgical technologies, in the heat treatment of materials, in the cultivation of single crystals, during freezing-thawing of soils, in electric welding, as well as in a number of other fields of science and practice. For the mathematical description of such thermal, diffusion and thermodiffusion processes, accompanied by phase transformations and the absorption or release of latent heat, single-phase or two-phase Stefan models are used [1-4]. The main feature of the Stefan model is that the phase boundary moving in time, which creates time-varying regions in which the determination of temperature fields or concentration of substances is required, is not set a priori and must be determined during the solution process. The questions of the existence and uniqueness of the solution of single-phase and two-phase Stefan problems are studied in [5]. Currently, a large number of analytical and numerical methods for studying the single-phase and two-phase Stefan model are known [6-10].

It should be noted that the efficiency of many technological processes, where heat transfer with phase transformation takes place, largely depends on the law of movement of the movable phase interface. In this regard, the task of regulating the movement of the phase interface in the processes of heat transfer with phase transformation is very important. In this paper, on the example of the ice melting process, the

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problem of regulating the movement of the interface is presented as a boundary inverse problem [11,12] for the single-phase Stefan model.

The general theory and applications of numerical methods for solving boundary inverse problems are discussed in [11–14]. It should be noted that the questions of the existence and uniqueness of the solution of boundary inverse problems were studied in [15, 16]. In [17], similar questions were investigated for various types of inverse problems of the single-phase and two-phase Stefan model. Currently, there is an extensive literature on numerical methods for solving inverse Stefan problems [18–20]. However, most of these papers are devoted to coefficient inverse problems and problems about sources, where the gradient iterative method is mainly used. In this paper, a non-iterative computational algorithm is proposed to solve the inverse problem.

PROBLEM STATEMENT

Let us consider a one-dimensional block of ice with a length l at the melting temperature of the ice T_* . From the moment of time t = 0, the block from the border x = 0 is heated under the temperature f(t), $f(t) > T_*$. As a result, the process of melting ice begins and a melting zone [0, s(t)] with a movable boundary s(t) is formed, and $\frac{ds}{dt} > 0$, t > 0, i.e., the melting zone expands over time. Consequently, the ice block is divided into thawed and frozen zones corresponding to different aggregate states. It is assumed that the mobile interface of the frozen and thawed zone s(t) has a melting point of ice. Assume that the temperature in the frozen zone [s(t), l] is equal to the melting temperature of ice T_* . Then the mathematical description of the ice melting process under consideration can be presented in the form of a single-phase Stefan model [1-4], which includes a thermal conductivity equation describing the temperature change in the melt zone

$$\frac{\partial T}{\partial t} = \chi \frac{\partial^2 T}{\partial x^2}, \quad (x, t) \in \Omega_s = \{0 < x < s(t), \quad 0 < t \le t_*\}, \tag{1}$$

a condition on a fixed boundary describing the temperature change over time on the boundary of the block

$$T(0, t) = f(t), \ 0 < t \le t_*,$$
(2)

Stefan's condition, which determines the speed of movement of the movable boundary 2T(r(t), t)

$$wp \frac{ds}{dt} = -\lambda \frac{\partial T(s(t), t)}{\partial x}, \ 0 < t \le t_*,$$
(3)

condition on the movable boundary between the thawed and frozen zone

$$T(s(t), t) = T_*, \ 0 < t \le t_*, \tag{4}$$

initial temperature distribution

$$T(x,0) = T_*,$$
 (5)

where T(x, t) is the temperature in the melt zone, w is the specific latent heat of melting, λ, ρ , χ is the coefficient of thermal conductivity, density and coefficient of thermal conductivity in the melt zone.

It should be noted that the direct problem for the model (1)–(5) consists in finding functions T(x, t) and s(t) satisfying equations (1), (3) with given coefficients χ , λ , ρ , w and additionally given conditions (2), (4), (5). However, in practice, for many thermal, diffusion processes accompanied by phase transformations, tasks are very important in which those boundary conditions are determined in which the

movement of the movable boundary is ensured according to a predetermined law. In this regard, within the framework of model (1)–(5), we set the following inverse problem: find such an ice heating mode on the border of the block that would ensure the movement of the movable boundary between the thawed and frozen zone according to a given law.

Thus, the law of moving the movable boundary s(t) is considered to be known and it is required to determine the functions T(x, t) and f(t) from equation (1) and additional conditions (2)–(5). Since the unknown problems are functions T(x, t) and f(t), therefore, problem (1)–(5) belongs to the class of boundary inverse problems [11–14].

METHOD FOR SOLVING THE PROBLEM

Assuming the existence and uniqueness of the solution of the inverse problem (1)–(5), we transform it using the method of straightening the fronts [4]. To this end, we introduce variable substitutions

$$y = \frac{x}{s(t)}, t = t, T(x, t) = T(y, t)$$

It is obvious that in this case the Ω_s area of setting equation (1) is uniquely mapped to the area $\Omega = \{0 < y < 1, 0 < t \le t_*\}$. Then equation (1) and additional conditions (2)–(5) in the new variables take the form

$$\frac{\partial T}{\partial t} = d(t)\frac{\partial^2 T}{\partial y^2} + r(y,t)\frac{\partial T}{\partial y},\tag{6}$$

$$(y, t) \in \Omega = \{0 < y < 1, \ 0 < t \le t_*\}, \quad T(0, t) = f(t), \ 0 < t \le t_*,$$
(7)

$$\frac{\partial T(1,t)}{\partial y} = v(t), \ 0 < t \le t_*, \tag{8}$$

$$T(1, t) = T_*, \ 0 < t \le t_*,$$
 (9)

$$T(y,0) = T_*,$$
 (10)

where $d(t) = \frac{\chi}{s^2(t)}$; $r(y, t) = \frac{y}{s(t)} \frac{ds}{dt}$; $v(t) = -\frac{s(t)w\rho}{\lambda} \frac{ds}{dt}$.

The advantage of such a transformation is that the computational domain of the problem (6)–(10) Ω becomes a rectangular area with fixed boundaries.

For the numerical solution of the boundary inverse problem (6)–(10), we construct its discrete analogue using the finite difference method. To do this, we introduce a uniform difference grid

$$\overline{\omega} = \{(y_i, t_j): y_i = i\Delta y, t_j = j\Delta t, i = 0, 1, 2, \dots n, j = 0, 1, 2, \dots m\}$$

in a rectangular area $\Omega = \{0 < y < 1, 0 < t \le t_*\}$ with $\Delta y = 1/n$, variable y and $\Delta t = t_* / m$ time steps. The discrete analogue of the problem (6)–(10) on the grid $\overline{\omega}$ is represented as the following implicit difference scheme

$$\frac{T_i^{j} - T_i^{j-1}}{\Delta t} = d^{j} \frac{T_{i+1}^{j} - 2T_i^{j} + T_{i-1}^{j}}{\Delta y^2} + r_i^{j} \frac{T_{i+1}^{j} - T_i^{j}}{\Delta y},$$
(11)

$$i = 1, 2, ..., n - 1, j = 1, 2, ...m,$$

$$T_0^{\ j} = f^{\ j},$$
 (12)

$$\frac{T_n^{\ J} - T_{n-1}^{\ J}}{\Delta y} = v^{\ j},\tag{13}$$

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$$T_n^j = T_*,$$
 (14)

$$T_i^0 = T_*, \tag{15}$$

where $T_i^j \approx T(x_i, t_j)$, $r_i^j = r(y_i, t_j)$, $d^j = d(t_j)$, $f^j \approx f(t_j)$, $v^j = v(t_j)$. It should be noted that the difference problem (11)–(15) on the solution of the

original differential problem (6)–(10) has the first order of approximation in Δy and Δt . The resulting difference problem is a system of linear algebraic equations in which the approximate values of the desired functions T(y, t) and f(t) in the nodes of the difference grid $\overline{\omega}$ act as unknowns, i.e. T_i^{j} , f^{j} , i=0, 1, 2, ..., n, j=1, 2, 3, ..., m.

To split the system of difference equations (11)–(15) into mutually independent subsystems, each of which can be solved independently, the solution of this system for each fixed value j = 1, 2, ..., m is represented as [12, 21]

$$T_i^{\ j} = u_i^j + f^{\ j} p_i^j, \ i = 0, 1, 2, ..., n,$$
(16)

where u_i^j , p_i^j are unknown variables.

Substituting the expression T_i^{j} into equation (11), we get

$$\frac{u_i^j + f^j p_i^j - T_i^{j-1}}{\Delta t} = d^j \frac{u_{i+1}^j + f^j p_{i+1}^j - 2u_i^j - 2f^j p_i^j + u_{i-1}^j + f^j p_{i-1}^j}{\Delta y^2} + r_i^j \frac{u_{i+1}^j + f^j p_{i+1}^j - u_i^j - f^j p_i^j}{\Delta y}$$

or

$$\left[\frac{u_i^j - T_i^{j-1}}{\Delta t} - d^j \frac{u_{i+1}^j - 2u_i^j + u_{i-1}^j}{\Delta y^2} - r_i^j \frac{u_{i+1}^j - u_i^j}{\Delta y}\right] + f^j \left[\frac{p_i^j}{\Delta t} - d^j \frac{p_{i+1}^j - 2p_i^j + p_{i-1}^j}{\Delta y^2} - r_i^j \frac{p_{i+1}^j - p_i^j}{\Delta y}\right] = 0$$

A substitution expression T_i^{j} in (12), (13) gives

$$u_0^j + f^j p_0^j = f^j, \quad \frac{u_n^j - u_{n-1}^j}{\Delta y} + f^j \frac{p_n^j - p_{n-1}^j}{\Delta y} = v^j.$$

From the presented relations we obtain the following difference problems for determining auxiliary variables u_i^j , p_i^j , i = 0, 1, 2, ..., n, for each fixed value j, i = 1, 2, ..., m,

$$\frac{u_i^j - T_i^{j-1}}{\Delta t} - d^j \frac{u_{i+1}^j - 2u_i^j + u_{i-1}^j}{\Delta y^2} - r_i^j \frac{u_{i+1}^j - u_i^j}{\Delta y} = 0,$$
(17)

$$\iota_0^j = 0, (18)$$

$$\frac{u_n^j - u_{n-1}^j}{\Delta v} = v^j.$$
 (19)

$$\frac{p_i^j}{\Delta t} - d^j \frac{p_{i+1}^j - 2p_i^j + p_{i-1}^j}{\Delta y^2} - r_i^j \frac{p_{i+1}^j - p_i^j}{\Delta y} = 0,$$
(20)

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$$p_0^j = 1,$$
 (21)

$$\frac{p_n^j - p_{n-1}^j}{\Delta y} = 0,$$
 (22)

j = 1, 2, ..., m.

The difference problems (17)–(19) and (20)–(22) for each fixed value *j*, j = 1, 2, ..., m, are a system of linear algebraic equations with a tridiagonal matrix and solutions of these systems can be found by the Thomas method [12]. And substituting representation (16) into (14), we will have

$$u_n^j + f^j p_n^j = T_*.$$

From here we obtain a formula for determining the approximate value of the desired function f(t) at $t = t_j$, i.e. f^{j}

$$f^{j} = \frac{T_{*} - u_{n}^{j}}{p_{n}^{j}}, \ j = 1, 2, 3, ..., m.$$
(23)

Thus, the computational algorithm for solving the difference problem (11)–(15) by definition T_i^{j} , f^{j} , i = 0, 1, 2, ..., n, on each time layer j, j = 1, 2, ..., m, consists of the following stages:

• solutions of two independent difference problems (17)–(19) and (20)–(22) with respect to auxiliary variables u_i^j , p_i^j , i=0, 1, 2, ..., n, are determined;

• the formula (23) determines the approximate value of the desired function f(t) at $t = t_j$, i.e. f^{j} ;

• the values of variables T_i^{j} are calculated according to the formula (16).

It should be noted that the applicability of the proposed computational algorithm is associated with the fulfillment of the condition

$$p_n^J \neq 0, \ j = 1, 2, 3, ..., m.$$
 (24)

To check condition (24), we find an explicit formula for calculating p_n^j . To this end, we first transform the system (20)–(22) into the form

$$a_i p_{i-1}^j - c_i p_i^j + b_i p_{i+1}^j = 0, \ i = 1, 2, ..., n-1,$$
(25)

$$p_0^j = 1,$$
 (26)

$$p_n^j = p_{n-1}^j \,, \tag{27}$$

$$j = 1, 2, ..., m$$
,

where $a_i = \frac{d^j}{\Delta y^2}$, $b_i = \frac{d^j}{\Delta y^2} + \frac{r_i^J}{\Delta y}$, $c_i = a_i + b_i + \frac{1}{\Delta t}$.

The system of equations (25)–(27) has a tridiagonal matrix and according to the Thomas method, its solution for each fixed value j = 1, 2, 3, ..., m can be represented as

$$p_{i+1}^{j} = \alpha_{i+1} p_{i}^{j} + \beta_{i+1}, \quad i = 0, 1, 2, ..., n-1,$$
(28)

where $\alpha_i = \frac{a_i}{c_i - \alpha_{i+1}b_i}$, $\beta_i = \frac{b_i\beta_{i+1}}{c_i - \alpha_{i+1}b_i}$, $i = n - 1, n - 2, ..., 1, \alpha_n = 1, \beta_n = 0$.

We will write the representation (28) when i = n - 1:

$$p_n^J = \alpha_n p_{n-1}^J + \beta_n.$$

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Substituting here the representation for p_{n-1}^{j} , i.e. $p_{n-1}^{j} = \alpha_{n-1}p_{n-2}^{j} + \beta_{n-1}$, we have

$$p_n^j = \alpha_n \alpha_{n-1} p_{n-2}^j + \alpha_n \beta_{n-1} + \beta_n.$$

Further, substituting the corresponding representations p_{n-2}^j , p_{n-3}^j , ..., p_1^j into the last equation, we obtain an explicit formula for calculating p_n^j :

$$p_n^j = p_0^j \prod_{i=1}^n \alpha_i + \sum_{i=1}^{n-1} \beta_i \prod_{k=i+1}^n \alpha_k + \beta_n.$$

But a simple analysis taking into account $a_i > 0$, $b_i > 0$, $c_i > a_i + b_i$, $i = \overline{1, n-1}$, shows that

$$0 < \alpha_i = \frac{a_i}{c_i - \alpha_{i+1}b_i} = \frac{a_i}{(c_i - a_i - b_i) + a_i + (1 - \alpha_{i+1})b_i} < 1, \ \beta_i = 0, \ i = \overline{1, n-1}.$$

As a result, for the calculation p_n^j we finally get

$$p_n^j = p_0^j \prod_{i=1}^n \alpha_i.$$

It follows that $p_n^j \neq 0$, j = 1, 2, 3, ..., m.

RESULTS OF NUMERICAL CALCULATIONS

To test the effectiveness of the practical application of the proposed computational algorithm, the following model problem is considered:

— according to a given law of motion of a moving boundary $s(t) = \beta \sqrt{t}$, find functions T(x, t) and f(t) satisfying the following conditions:

$$\frac{\partial T}{\partial t} = \chi \frac{\partial^2 T}{\partial x^2}, \ 0 < x < s(t), \qquad 0 < t \le t_*,$$
$$T(0, t) = f(t), \ 0 < t \le t_*,$$
$$-\lambda \frac{\partial T(s(t), t)}{\partial x} = wp \frac{ds}{dt}, \ 0 < t \le t_*,$$
$$T(s(t), t) = T_*, \ 0 < t \le t_*.$$

This problem has an exact solution

$$f(t) = \text{const} = \bar{f}, \quad T(x, t) = T_0 + (T_* - T_0) \frac{\int_0^{x/2\sqrt{\chi t}} e^{-\xi^2} d\xi}{\int_0^{\beta/2\sqrt{\chi}} e^{-\xi^2} d\xi},$$

where the magnitude β is the root of the nonlinear equation

$$\beta = \frac{\lambda}{wp\sqrt{\chi}} \frac{(T_0 - T_*)}{\int\limits_0^{\beta/2} \sqrt{\chi}} e^{-\frac{\beta}{4\chi}} \cdot \int_0^{2\pi/2} e^{-\frac{\beta}{4\chi}} d\xi$$

Based on the proposed computational algorithm, the numerical solution of the model problem under consideration is determined. Numerical calculations were per-

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<u> </u>	~										
	f(t)										
t	$\overline{f} = 5,$ s(t) = $= 129 \cdot A$	$\overline{f} = 10,$ s(t) = $= 181 \cdot A$	$\overline{f} = 15,$ s(t) = $= 220 \cdot A$	$\overline{f} = 20,$ s(t) = $= 252 \cdot A$	$\overline{f} = 25,$ s(t) = $= 279 \cdot A$	$\overline{f} = 30,$ s(t) = $= 303 \cdot A$	$\overline{f} = 35,$ s(t) = $= 325 \cdot A$	$\overline{f} = 40,$ s(t) = $= 345 \cdot A$	$\overline{f} = 45,$ s(t) = $= 363 \cdot A$	$\overline{f} = 50,$ s(t) = $= 380 \cdot A$	
1	5.074	10.379	15.910	21.630	27.417	33.405	39.681	46.118	52.572	59.299	
2	4.998	9.960	14.966	19.953	24.822	29.689	34.622	39.516	44.267	49.066	
3	4.994	9.970	15.000	20.031	24.969	29.938	35.011	40.087	45.061	50.136	
4	4.994	9.970	14.992	20.028	24.964	29.927	34.990	40.052	45.007	50.057	
5	4.994	9.970	14.992	20.028	24.964	29.927	34.991	40.054	45.010	50.061	
6	4.994	9.970	14.992	20.028	24.964	29.927	34.991	40.054	45.010	50.061	
7	4.994	9.970	14.992	20.028	24.964	29.927	34.991	40.054	45.010	50.061	
8	4.994	9.970	14.992	20.028	24.964	29.927	34.991	40.054	45.010	50.061	
9	4.994	9.970	14.992	20.028	24.964	29.927	34.991	40.054	45.010	50.061	
10	4.994	9.970	14.992	20.028	24.964	29.927	34.991	40.054	45.010	50.061	

Table 1. Calculated values of f(t) for given s(t)

formed for the following values of variables; $T_* = 0^{\circ} C$; $\rho = 999.8 \text{ kg/m}^3$; $\lambda=0.569 \text{ W/(m °C)}$; $\chi = 13.5 \cdot 10^{-8} \text{ m}^2/\text{s}$; $w = 3.335 \cdot 10^5 \text{ J/kg}$. The results of numerical calculations carried out under various laws of motion of the movable boundary are presented in Table 1; in it *t* is the time, \bar{f} is the exact values, and $\tilde{f}(t)$ is the calculated values of the function f(t), $A = 10^{-6} t^{1/2}$.

From Table 1 it follows that during the first 5 seconds a certain constant temperature is set on the border of the block x = 0 and this temperature is taken to solve this problem. At the same time, the relative error of restoring the temperature regime at the border in all variants does not exceed 0.5%. The results of numerical calculations confirm that the constant temperature regime on the border of the block ensures the movement of the movable border according to the law $s(t) = \beta \sqrt{t}$.

CONCLUSIONS

Within the framework of Stefan's single-phase model, the inverse problem of melting a one-dimensional block of ice is considered, which consists in identifying the heating mode at a fixed boundary according to a given law of motion of the movable boundary. The proposed computational algorithm, based on the use of the method of rectification of fronts, discretization of the problem and the use of a special representation for solving a discrete problem, allows us to consistently determine the heating temperatures at a fixed boundary and the temperature distribution in the melt zone in each time layer. The proposed computational algorithm can be used in the study of the single-phase Stefan model.

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ІДЕНТИФІКАЦІЯ ГРАНИЧНОГО РЕЖИМУ В ОДНІЙ ТЕПЛОВІЙ ЗАДАЧІ НА ОСНОВІ ОДНОФАЗНОЇ МОДЕЛІ СТЕФАНА

Анотація. Розглянуто процес плавлення одномірного льодового блоку шляхом нагрівання його з лівої межі. Для математичного опису процесу плавлення запропоновано одновимірну однофазну модель Стефана, яка описує зміну температури в утворюваній талій зоні з рухомою межею. В межах цієї моделі поставлено задачу ідентифікації режиму нагріву на лівій межі блоку, який забезпечує переміщення рухомої межі талої зони за заданим законом. Поставлена обернена задача для однофазної моделі Стефана належить класу граничних обернених задач. Методом спрямлення фронтів область задачі з рухомою межею перетворено на область з фіксованими межами. Побудовано дискретний аналог оберненої задачі з використанням методу кінцевих різницевої задачі. В результаті різницева задача для кожного дискретного значення часової змінної ділиться на дві незалежні різницеві задачі другого порядку, для розв'язання яких застосовано абсолютно стійкий метод Томаса та лінійне рівняння відносно наближеного значення температури нагріву на лівій межі блоку. На основі запропонованого обчислювального алгоритму проведено числові експерименти.

Ключові слова: теплоперенесення з фазовим перетворенням, процес плавлення льоду, рухома межа поділу фаз, метод спрямлення фронтів, гранична обернена задача, різницевий метод.

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