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NUMERICAL METHOD FOR SOLVING THE STEFAN PROBLEM WITH EXPLICIT ISOLATION OF PHASE BOUNDARIES IN A MULTIPHASE DIFFUSION SYSTEM

ЧИСЛОВИЙ МЕТОД РОЗВ'ЯЗАННЯ ЗАДАЧІ СТЕФАНА З ЯВНИМ ВИДІЛЕННЯМ ГРАНИЦЬ РОЗДІЛУ ФАЗ У БАГАТОФАЗНІЙ ДИФУЗІЙНІЙ СИСТЕМІ

With the development of computational techniques and advancements in modeling physicochemical processes, methods for increasing the accuracy and simplifying algorithms and methods for calculating mathematical models have become increasingly important.

This work is devoted to the Stefan problem, to which problems of heat transfer with a liquid-solid phase transition and diffusion mass transfer with phase transformations in a solid (decomposition of solid solutions, deposition of diffusion coatings) are reduced. The features of numerical modeling of the Stefan problem in multiphase systems are considered.

The possibilities and shortcomings of existing numerical methods for solving this problem are analyzed.

A new numerical method for solving the Stefan problem in multiphase systems is proposed. This method is based on an implicit finite difference scheme and employs a nonlinear function approximation of the diffusant gradient directly at the moving phase interfaces. It is shown that this method helps to minimize the error in calculating the concentration gradient at the moving phase interfaces, where the grid function undergoes a first-order discontinuity, significantly simplifying the numerical solution algorithm for this problem.

A comparison of the proposed algorithm with existing numerical methods was carried out on a model problem of reactive diffusion in a solid, which is a Stefan problem in multiphase systems, using boundary and initial conditions that allow for its analytical solution.

***Keywords**: Stefan problem, numerical methods, phase boundary, finite difference scheme, explicit isolation of a moving boundary.*

З розвитком обчислювальної техніки і прогресом в області моделювання фізико-хімічних процесів особливої актуальності набувають способи підвищення точності та спрощення алгоритмів і методів розрахунку математичних моделей.

Дана робота присвячена проблемі Стефана, до якої зводяться завдання теплопереносу з фазовим переходом рідина - тверде тіло і дифузійного масопереносу з фазовими перетвореннями в твердому тілі (розпад твердих розчинів, нанесення дифузійних покриттів). Розглянуто особливості чисельного моделювання задачі Стефана в багатофазних системах.

Проаналізовано можливості та недоліки існуючих чисельних методів вирішення цього завдання.

Запропоновано новий чисельний метод розрахунку задачі Стефана в багатофазних дифузійних системах, який ґрунтується на неявній різницевій схемі. Метод використовує апроксимацію градієнта дифузанта нелінійною функцією безпосередньо біля рухомих міжфазних границь. Наведено, що цей метод сприяє мінімізації помилки розрахунку градієнта концентрації на рухливих міжфазних границях, де сіткова функція зазнає розрив першого роду. Це істотно впливає на точність розрахунку руху між фазних границь, що має суттєве значення при розв'язанні задач Стефана в багатофазних системах.

Порівняння запропонованого алгоритму з існуючими чисельними методами проводилося на модельній задачі реакційної дифузії в твердому тілі, що є задачею Стефана в багатофазних системах, з використанням граничних і початкових умов, які допускають її аналітичне рішення.

Наведено, що реальний розподіл концентрації елемента насичення в усіх шарах фаз дифузійного покриття є функцією, подібною erf-функції від координат. Внаслідок цього, при обчисленні градієнтів концентрації на рухомих границях розділу фаз, при використанні лінійної апроксимації похідних, на кожному кроці за часом виникає помилка. Ця помилка є системною і неминучою під час рішення задачі Стефана чисельними методами з явним виділенням границі фаз. Помилка обчислення градієнтів носить постійний характер, що призводить до системного збільшення швидкості руху границі на кожному часовому кроці розрахунку.

Розроблено спосіб мінімізації помилки апроксимації градієнта з використанням нелінійної апроксимуючої erf-функції, який дозволяє збільшити точність апроксимації градієнту до порядку (h^2, τ).

Розрахунки показали, що запропонований метод має точність, яка не перевищує 0,15 %.

***Ключові слова**: задача Стефана, чисельні методи, межа розділу фаз, різницева схема, явне виділення рухомої границі.*

Problem's Formulation

Numerical solutions of Stefan problems have seen widespread adoption of grid-based methods relying on implicit finite difference schemes. These schemes exhibit unconditional stability for any temporal and spatial step sizes, allowing for the unrestricted use of kinetic coefficients.

The primary challenge in solving such problems lies in the variable domain of the function (temperature for heat conduction, concentration for diffusion). The boundaries of this domain and their evolution over time are not known a priori.

The crux of the problem is the movement of the phase interface. As this interface moves, a node in the spatial grid disappears from one phase and appears in the neighboring phase. This renders the grid function undefined at this node, as it lacks a history in the new phase at the previous time step. Consequently, the finite difference approximation of derivatives involving this node cannot be formulated without additional assumptions.

Furthermore, the velocity of the phase interface, which is determined by the grid function values near the interface, in turn influences these values. At each time step, this velocity must be con-

sistent with the local grid function values. Any errors, whether random or systematic, in calculating the grid function or the phase interface position will propagate and diminish the accuracy of the results.

The distinctions between various finite difference-based solution methods stem from the approaches employed to address these challenges.

Analysis of recent research and publications

Existing analytical methods for solving problems with moving phase boundaries are limited to a very narrow class, typically involving idealized boundary conditions and one-dimensional problem formulations.

As previously mentioned, finite difference methods have gained the most popularity in the numerical modeling of Stefan problems. Depending on the type of numerical approximation of spatial derivatives, difference schemes can be divided into two classes: explicit difference schemes and implicit difference schemes.

Examples of using explicit difference schemes to solve heat and mass transfer problems are the methods proposed by Crank and Nicolson in the 1960s. In these methods, unknown grid functions T_k (or C_k for diffusion) and $\Gamma(t_n+1)$ at the new (n+1)th time layer were included only in the approximation of time derivatives.

As shown in the works of A.A. Samarskii on the theory of difference schemes, this difference scheme is conditionally stable. That is, it is stable only for sufficiently small time steps and imposes rather stringent constraints on the kinetic parameters of the system due to the accumulation of errors during the computational process. This drawback proved to be so significant that it prevented the application of this method to solving practically important problems.

Implicit difference schemes have proven to be the most suitable in this sense. An implicit difference scheme does not accumulate a systematic error in calculations, as this difference scheme is absolutely stable for any values of time and spatial steps. It allows the use of kinetic coefficients without any restrictions, which significantly expands the scope of its application for solving specific practical problems. It is also suitable for solving problems where the grid function may have both first and second-order discontinuities at the phase boundary.

The main problem of applying the implicit difference scheme to problems related to phase transformations, which lead to the movement of phase boundaries, lies in the variable geometry of the phases. When the phase boundary moves, a node of the spatial grid disappears in one of the neighboring phases, and a new node appears in the other, which previously belonged to the neighboring phase. The uncertainty of the grid function due to the lack of history in this phase at the previous time layer leads to the fact that the difference approximation of derivatives, which include this node of the spatial grid, cannot be written without additional assumptions.

Several authors have proposed various ways to overcome this difficulty.

As one way to eliminate the uncertainty of the function at a newly created node, B.M. Budak and A.A. Samarskii proposed methods related to smoothing the grid function near the moving boundary. The main idea of this group of methods was that the Stefan problem with moving phase boundaries was reduced to a problem of one-phase non-stationary heat conduction with fixed external boundaries. This method was used for heat conduction problems with phase transformations. Obviously, the temperature distribution function obtained as a result of calculations using these methods will be continuous in the entire domain of definition, at least with its first derivative. The main calculation error was most noticeable near the phase boundary, where the temperature function should have a second-order discontinuity. For the calculation of diffusion mass transfer problems, this method is generally unacceptable, since the concentration function of the diffusant in the matrix base undergoes a first-order discontinuity at the phase boundary.

The second group of methods is based on the fact that the time or spatial step was chosen in such a way that the phase boundary at each subsequent time layer fell into the node of the spatial grid. These are the so-called "boundary-following" methods. Examples of these methods can be found in the works of Baladi I.Y., Ayers D.L., Schoenhals R.I., and Gupta R.S., Kumar D.

It should be noted that the above methods also have a number of disadvantages. Firstly, this is the complexity of the computational process using iterative procedures. Secondly, the method is com-

pletely unsuitable for a multiphase system, since it is impossible to choose such a time or spatial step at which all the moving boundaries of the multiphase system will simultaneously fall into the nodes of the spatial grid.

Earlier, the authors proposed a method based on the use of an implicit difference scheme that allows determining the value of the function at a newly created node of the spatial grid without changing the time step. This is the "auxiliary grid" method [1]. The method allowed solving the aforementioned problems and could be applied not only to a multiphase diffusion system but also used to solve the problem in a multidimensional formulation.

However, all of the above numerical calculation methods, regardless of the accuracy of calculating the grid function, have a systematic error associated with determining the gradients near the moving phase boundary, since they use linear interpolation of the grid function. Although the function itself to the left and right of the moving phase boundary differs significantly from the linear one, especially at the initial moments of phase growth.

Formulation of the study purpose

The goal of this work is to develop a numerical method based on an implicit finite difference scheme, specifically designed for modeling diffusion processes in multiphase systems with moving phase boundaries.

The essence of the development lies in minimizing the error in calculating the concentration gradient near the moving phase boundary by using a nonlinear approximating function. This, in turn, will allow optimizing the calculation scheme, increasing its accuracy and ensuring the possibility of applying such an algorithm to solve a wide range of problems related to the multiphase, multidimensional structure of the diffusion domain and a wide range of boundary conditions on the external boundaries of the diffusion system.

Presenting main material

To analyze the problem, let us consider a one-dimensional (planar) problem for a multiphase diffusion system with moving phase boundaries. An example of such a system is the process of diffusion saturation from the surface of a metal base matrix with a saturating element, which can form various intermetallic phases with the base metal.

Diffusion of the saturating element into the metal base matrix in the presence of several phases is described by a system of second-order partial differential equations based on Fick's second law:

$$\frac{\partial C_q(x,t)}{\partial t} = \frac{\partial}{\partial x}\left(D_q(T, C_q)\frac{\partial C_q(x,t)}{\partial x}\right), \quad (1)$$

here: q = 1, 2, … Q — the phase number, starting from the outer surface x = 0; x, t — the current coordinate and time; $C_q(x,t)$ — concentration profile in the q-th phase; $D_q(T, C_q)$ — diffusion coefficient in the q-th phase (generally depends on the concentration of the diffusant and temperature); T — diffusion zone temperature.

The initial distribution of the diffusant concentration in each q-th phase can be arbitrary and given by a function:

$$C_q(x, 0) = \varphi_q(x). \quad (2)$$

Boundary conditions at the outer boundary and at the end of the diffusion zone (L is the length of the diffusion zone) can be written as follows:

$$C_1(0, t) = \varphi_1(t); \quad (3)$$

$$C_Q(L, t) = \varphi_2(t). \quad (4)$$

The system of equations (1)—(4) must be supplemented with boundary conditions and a mass balance equation at all internal moving boundaries:

$$C_q(x,t)|_{x=\Gamma_q(t)-0} = C_q^{q+1}(t); \quad (5)$$

$$C_{q+1}(x,t)|_{x=\Gamma_q(t)+0} = C_{q+1}^{q}(t); \quad (6)$$

$$-D_q(T, C_q)\frac{\partial C_q}{\partial x}|_{x=\Gamma_q} = -D_{q+1}(T, C_{q+1})\frac{\partial C_{q+1}}{\partial x}|_{x=\Gamma_q} + \left(C_q^{q+1}(t) - C_{q+1}^{q}(t)\right)\frac{d\Gamma_q}{dt}, \quad (7)$$

here: $\Gamma_q(t)$ — the interface between the q-th and (q+1)-th phases; $C_q^{q+1}(t)$ — concentration in the q-th phase at the interface with the (q+1)-th phase.

Thus, the system of equations (1)—(7) describes the evolution of the structure and composition of a multiphase diffusion system in the presence of Q moving interphase boundaries. It should be noted again that, in the general case, diffusion coefficients in all phases of the diffusion system may depend both on temperature (Arrhenius-type exponential dependence, using the activation energy Q_q: $D_{0q}\exp(Q_q/RT)$) and on the concentration of the diffusant in each phase — $D_q(T, C_q)$.

A more detailed description of this mathematical model can be found in [1].

In the Stefan diffusion problem, the position of the moving phase boundary is determined from the mass balance equation (7) for the diffusing element at this boundary Γ_q. Since the fluxes of the diffusing element are determined by the gradients of its concentration, the accuracy of determining concentrations near the moving boundary and the accuracy of the finite-difference approximation of the first derivative affect the accuracy of determining the position of the interphase boundary Γ_q.

The traditional finite difference approximation of the diffusion equation in regular nodes of a uniform grid for one-, two-, and three-dimensional problems is carried out with an accuracy of order $\mathbf{(h^2,\tau)}$ [2], where **h** — is the spatial grid step and **τ** — is the time step. In the case of explicit phase boundary tracking [3,4], there is always a boundary node **ip′**, the distance δ from which to the moving boundary is less than the spatial grid step **δ < h** (Fig. 1). Therefore, the approximation of the diffusion equation at this node is carried out on a non-uniform grid, which leads to a decrease in accuracy to the order of **(h,τ)**.

Thus, the numerical solution of the diffusion equation within a single phase can give the largest errors in the values of the diffusant element concentration near the moving boundary, which will subsequently affect the accuracy of determining the coordinate Γ_q of this boundary.

In most works devoted to the numerical modeling of reactive diffusion with explicit phase boundary tracking, the finite difference approximation of gradients in the balance equation (7) at the moving boundary is carried out using a two-point scheme, which includes the boundary node and the phase boundary itself [5,6,7]. The accuracy of such an approximation of the first derivative is found to be of the order of **(h,τ)**, which is consistent with the accuracy of the finite difference approximation of the diffusion equation at the boundary node.

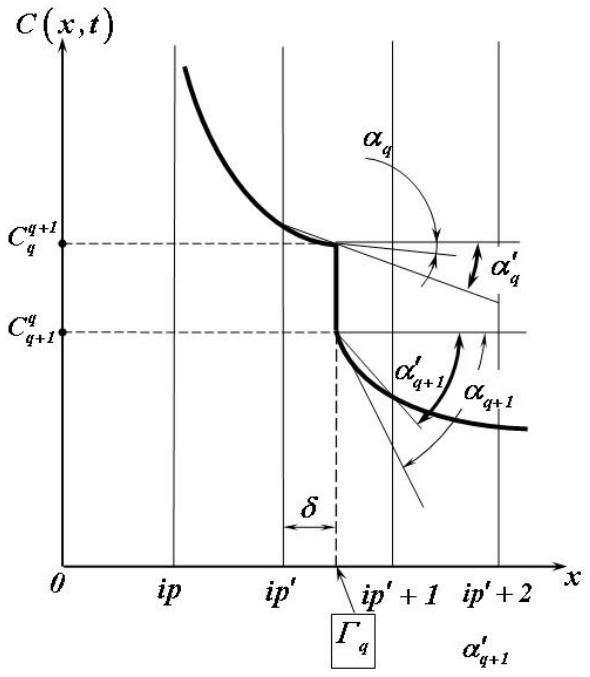

Fig. 1. Emergence of a systematic error in gradient calculation: α_q , α_{q+1} — analytical values of tangent angles to the function; α'_q , α'_{q+1} — tangent angles calculated using finite difference approximation of gradients

This work is dedicated to investigating possibilities for improving the accuracy of determining the position of the phase boundary without significantly complicating the calculation algorithm or reducing its execution speed.

Systematic errors in gradient approximation and methods for their elimination

The use of an implicit scheme for calculating the concentration of the diffusing element within a single phase suppresses any random errors that may arise during the calculation process and should not lead to the accumulation of errors at the boundary node. It is known that the actual distribution of the diffusing element's concentration within a single phase is a concave continuous function of coordinates. Therefore, the two-point scheme approximation of the first derivative always gives a slightly overestimated value of the gradient (Fig. 1) in the phase with a higher concentration of the diffusing element and slightly underestimates the gradient in the phase with a lower concentration of the diffusing element.

Such systematic errors in the calculation of gradients lead (Fig. 1) to an increase in the

velocity V_{Γ_q} of the moving interface $V_{\Gamma_q} = \frac{d\Gamma_q}{dt}$; (Γ_q is the coordinate of the interphase boundary).

Let us demonstrate this.

Fig. 1 shows a schematic diagram of the concentration dependence of the diffusing element a in the phases around the moving interphase boundary. Here, α_q and α_{q+1} — are the analytical values of the tangent angles at the interphase boundary at points $x=\Gamma_q-0$ and $x= x=\Gamma_q+0$, respectively. And α'_q , α'_{q+1} — are the values of the tangent angles of the segments at the interphase boundary, which are used in the process of finite-difference approximation of gradients.

It is evident that the following inequalities will always hold: $\alpha'_q > \alpha_q$ and $\alpha'_{q+1} < \alpha_{q+1}$. Consequently, the finite difference approximation results in a diffusion flux of element A towards the phase interface that is always greater than the actual flux. Similarly, the flux of element A away from the phase interface is always less than the actual flux, leading to an overestimation of the phase boundary movement velocity.

As the actual concentration distribution of the diffusing element approaches a linear profile, the errors in gradient calculation decrease, and the velocity of the phase boundary movement converges to the analytical value. The systematic error in gradient approximation at the phase interface can be reduced in two ways:

1) by using nonlinear approximating functions;

2) by increasing the accuracy of gradient approximation through a finer spatial grid.

Increasing the spatial grid points always leads to a significant increase in computational load and, consequently, an increase in computation time.

Therefore, we will first consider the use of nonlinear approximating functions.

Minimization of gradient approximation error using a nonlinear approximating function

All existing analytical solutions to the diffusion equation demonstrate that the concentration distribution of the diffusing element is described by *erf* or *erfc* - functions, as exemplified in [2]:

$$C(x,t) = C_0\, erfc\left(\frac{x}{2\sqrt{D_q t}}\right) = C_0 - C_0\, erf\left(\frac{x}{2\sqrt{D_q t}}\right);$$

$$C_q(x,t) = C_q^{q-1} - (C_q^{q-1} - C_q^{q+1})\,\frac{erf\left(\frac{x}{2\sqrt{D_q t}}\right) - erf\left(\frac{\beta_{q-1}}{\sqrt{D_q}}\right)}{erf\left(\frac{\beta_q}{\sqrt{D_q}}\right) - erf\left(\frac{\beta_{q-1}}{\sqrt{D_q}}\right)}\ .$$

Typically, at any point in time, these functions can be represented by: $y(x)=m-a\ erf(\sqrt{b}\cdot x)$. In this equation, *m*, *a*, and *b* — represent constants.

Let us find the derivative of this function at the point $x = \Gamma_q-0$, that is, from the left side of the boundary Γ_q.

We have:

$$\left.\frac{\partial y}{\partial x}\right|_{\Gamma_q - 0} = -a_L \cdot \frac{2\sqrt{b_L}}{\sqrt{\pi}} \cdot \exp\,(-b_L x^2), \tag{8}$$

here, the subscript L stands for 'left', meaning from the left side of the boundary Γ_q.

Considering the Lagrange's mean value theorem and the known concentration values C_q^{q+1} of the diffusing element (Fig. 1) at the moving boundary Γ_q and the nearest grid nodes ***ip*** and ***ip′***, let us write a two-point finite difference approximation of the gradients on the segments (***ip′*** - Γ_q) and (***ip*** - ***ip′***) to determine the unknown constants $\boldsymbol{a_L}$ and $\boldsymbol{b_L}$:

$$\frac{C_q^{q+1} - C_{ip'}}{\Gamma_q - x_{ip'}} = a_L \cdot \frac{2\sqrt{b_L}}{\sqrt{\pi}} \cdot \exp\,(-b_L x_1^2); \tag{9}$$

$$\frac{C_{ip'} - C_{ip}}{x_{ip'} - x_{ip}} = a_L \cdot \frac{2\sqrt{b_L}}{\sqrt{\pi}} \cdot \exp\,(-b_L x_2^2), \tag{10}$$

here, x_1 and x_2 — are some points located inside the intervals $\Gamma_q - x_{ip'}$ and $x_{ip'} - x_{ip}$, respectively.

Considering that the concentration distribution function within a single phase is a monotonic smooth function, it can be assumed that the points $\boldsymbol{x_1}$ and $\boldsymbol{x_2}$ are approximately in the middle of the corresponding intervals and the following relations hold:

$$x_1 = \frac{\Gamma_q + x_{ip'}}{2} \quad x_2 = \frac{x_{ip'} + x_{ip}}{2}. \tag{11}$$

Substituting (11) into (9) and (10), we obtain:

$$\frac{C_q^{q+1}-C_{ip'}}{\Gamma_q-x_{ip'}} = a_L \cdot \frac{2\sqrt{b_L}}{\sqrt{\pi}} \cdot \exp\left(-b_L\left(\frac{\Gamma_q+x_{ip'}}{2}\right)^2\right);$$
$$\frac{C_{ip'}-C_{ip}}{x_{ip'}-x_{ip}} = a_L \cdot \frac{2\sqrt{b_L}}{\sqrt{\pi}} \cdot \exp\left(-b_L\left(\frac{x_{ip'}+x_{ip}}{2}\right)^2\right).$$

By solving the resulting system of equations with respect to $\boldsymbol{a_L}$ and $\boldsymbol{b_L}$, we arrive at the following expressions:

$$b_L = \frac{4\cdot\ln\left(\frac{\left(C_q^{q+1}-C_{ip'}\right)\cdot\left(x_{ip'}-x_{ip}\right)}{\left(C_{ip'}-C_{ip}\right)\cdot\left(\Gamma q-x_{ip'}\right)}\right)}{(x_{ip'}+x_{ip})^2-(\Gamma_q+x_{ip'})^2}; \quad (12)$$

$$a_L = -\frac{C_q^{q+1}-C_{ip'}}{\Gamma_q-x_{ip'}} \cdot \frac{\sqrt{\pi}}{2\sqrt{b_L}} \cdot \exp\left(b_L\left(\frac{\Gamma_q+x_{ip'}}{2}\right)^2\right). \quad (13)$$

Now, using equation (8) and taking into account equations (12) and (13), and considering $x = \Gamma_q$, we will calculate the first derivative at the phase boundary Γ_q.

After some simple transformations, we obtain:

$$\left.\frac{\partial y}{\partial x}\right]_{\Gamma_q-0} = \frac{C_q^{q+1}-C_{ip'}}{\Gamma_q-x_{ip'}} \cdot \exp\left(b_L\left(\left(\frac{\Gamma_q+x_{ip'}}{2}\right)^2-{\Gamma_q}^2\right)\right). \quad (14)$$

Expression (14) represents the value of the linear approximation of the first derivative to the left of the phase interface, multiplied by an exponential factor, whose exponent is always negative.

Thus, the overestimation of the first derivative value when it is approximated linearly will be compensated by multiplication by an exponential factor, whose value is always less than unity, and the overestimation of the first derivative will decrease, approaching the true value.

By performing similar reasoning, let us find the derivative of the function $y(x)=m_R-a_R\ erf(\sqrt{b_R}\cdot x)$ at the point $x = \Gamma_q+0$, that is, from the right side of the boundary Γq. Here, the subscript R means: on right, — "from the right side of the boundary Γq".

Finally, we obtain a system of equations for $\boldsymbol{a_R}$ and $\boldsymbol{b_R}$:

$$b_R = \frac{4\cdot\ln\left(\frac{\left(C_{q+1}^{q}-C_{ip'+1}\right)\cdot\left(x_{ip'+2}-x_{ip'+1}\right)}{\left(C_{ip'+2}-C_{ip'+1}\right)\cdot\left(\Gamma q-x_{ip'+1}\right)}\right)}{(x_{ip'+2}+x_{ip'+1})^2-(\Gamma_q+x_{ip'+1})^2};$$
$$a_R = -\frac{C_{q+1}^{q}-C_{ip'+1}}{\Gamma_q-x_{ip'+1}} \cdot \frac{\sqrt{\pi}}{2\sqrt{b_R}} \cdot \exp\left(b_R\left(\frac{\Gamma_q+x_{ip'+1}}{2}\right)^2\right).$$

Therefore, we finally arrive at:

$$\left.\frac{\partial y}{\partial x}\right]_{\Gamma_q+0} = \frac{C_{q+1}^{q}-C_{ip'+1}}{\Gamma_q-x_{ip'+1}} \cdot \exp\left(b_R\left(\left(\frac{\Gamma_q+x_{ip'+1}}{2}\right)^2-{\Gamma_q}^2\right)\right). \quad (15)$$

Expression (15) represents the value of the linear approximation of the first derivative to the right of the phase interface, multiplied by an exponential factor, whose exponent is always positive.

Since in this case $\Gamma_q < x_{ip'+1}$,, the exponential factor will be greater than unity, and the underestimated value of the first derivative will increase, approaching the true value.

Comparison of the accuracy of the proposed method for reducing the systematic error of gradient approximation

When recording the system of equations (1)—(7) using a finite difference scheme, it is necessary to use dimensionless quantities normalized to the **h** -spatial grid step and the **τ** -time grid step:

spatial variable — $\frac{x}{h}$ (determines the number of nodes of the spatial grid);

time variable — $\frac{t}{\boldsymbol{\tau}}$ (determines the number of time steps);

dimensionless diffusion coefficient — $\frac{D_q\boldsymbol{\tau}}{h^2}$ (dimensionless coefficient, normalized by the spatial step and time step).

This is due to the fact that when constructing a finite difference scheme, certain conditions must be met for building a spatial grid and determining the time step. In order to obtain a more or less accurate calculation, it is necessary to use at least several hundred spatial steps, and the time step

should be chosen so that the moving phase boundary does not cross more than one spatial grid node in one time step.

This is because constructing a finite difference scheme requires satisfying specific conditions for spatial grid and time step selection. To ensure reasonable accuracy, at least several hundred spatial steps are necessary. Moreover, the time step should be small enough to prevent the moving phase boundary from crossing more than one grid node per time step.

Consequently, the following dimensionless parameters were chosen for the model problem:

Constant concentration on the outer surface – $C_1^0(0,t) = 30$ %;

Concentration at the moving boundary in the 1st phase – $C_2^1 = 20$ %;

Concentration at the moving boundary in the 2nd phase – $C_1^2 = 10$ %;

Concentration at the inner surface of the diffusion zone – $C_2(L,t) = 0$;.

Dimensionless diffusion coefficient in the first phase ($\frac{D_1\tau}{h^2}$) – D1 = 2,3;

Dimensionless diffusion coefficient in the second phase ($\frac{D_2\tau}{h^2}$) – D2 = 0,992.

According to the definition of these dimensionless quantities, in the following, we will count time in time steps and distance in spatial steps.

The formulation of the Stefan problem in this form allows for an analytical solution. According to the analytical solution [1] of the problem (1)—(7), a parameter can be obtained that determines the position of the moving boundary $\boldsymbol{\Gamma = 2\beta\sqrt{t}}$, $\boldsymbol{\beta = const}$ (in this example, the calculated coefficient is $\boldsymbol{\beta}$ = 0.61477).

In order to avoid mathematical difficulties at the initial time t=0 in numerical calculations (in numerical modeling it is impossible to set zero phase thicknesses at the initial moment, in contrast to the analytical solution), the moment $\boldsymbol{t}$ = 25 steps was chosen as the initial moment, for which the position of the phase boundary and the concentration distribution in the phases were calculated using analytical formulas. These data provided the initial values for the phase thicknesses and concentration distribution for the grid function. Further numerical modeling was carried out using this distribution as the initial condition.

The most vivid indicator of the accuracy of the calculations is the dynamics of the phase boundary movement. The simulation results are presented in Tabl. 1.

Table 1. Dependence of the phase boundary coordinate on the time of the diffusion experiment

Time, number of time steps	Analytical solution Γ_A, number of spatial steps	Calculated values of Γ_1	Difference from analytical solution $\Delta\Gamma_1$	Relative error, %
27	6,38887725	6,39368705	0,00481	0,0753
29	6,62127554	6,622018989	0,000743	0,0112
31	6,84578899	6,844573	-0,00122	-0,0178
35	7,27405674	7,283902621	0,009846	0,1354
39	7,67847484	7,677959859	-0,00051	-0,0066
45	8,24800506	8,254162705	0,006158	0,0747
53	8,95118631	8,947650326	-0,00354	-0,0395
65	9,91286839	9,910290604	-0,00258	-0,0260
81	11,06586	11,06334033	-0,00252	-0,0228
105	12,5990358	12,59972307	0,000687	0,0055
137	14,3913967	14,39405031	0,002654	0,0184

Continue of the table 1

183	16,6329088	16,63614174	0,003233	0,0194
247	19,3237379	19,32880294	0,005065	0,0262
337	22,571354	22,57716654	0,005813	0,0258
463	26,4565468	26,46333595	0,006789	0,0257
639	31,0808646	31,08870524	0,007841	0,0252
885	36,5775234	36,58525803	0,007735	0,0211
1229	43,1041022	43,11216	0,008057	0,0187
1711	50,8589824	50,86675	0,007769	0,0153
2387	60,0715546	60,07925	0,007696	0,0128

As can be seen from Tabl. 1, the results of numerical calculations of Γ_1, the coordinate of the phase boundary, differ very little from the analytical solution GA. And the relative error does not exceed ε_{max} = 0,14 % compared to the analytical solution. On any graph, they will hardly be distinguishable.

Therefore, to analyze the change in the error during calculations, Fig. 2 shows the graphs of the time dependence of the difference between the calculated and analytical values of the phase boundary coordinate ($\Delta\Gamma_1 = \Gamma_1 - \Gamma_A$).

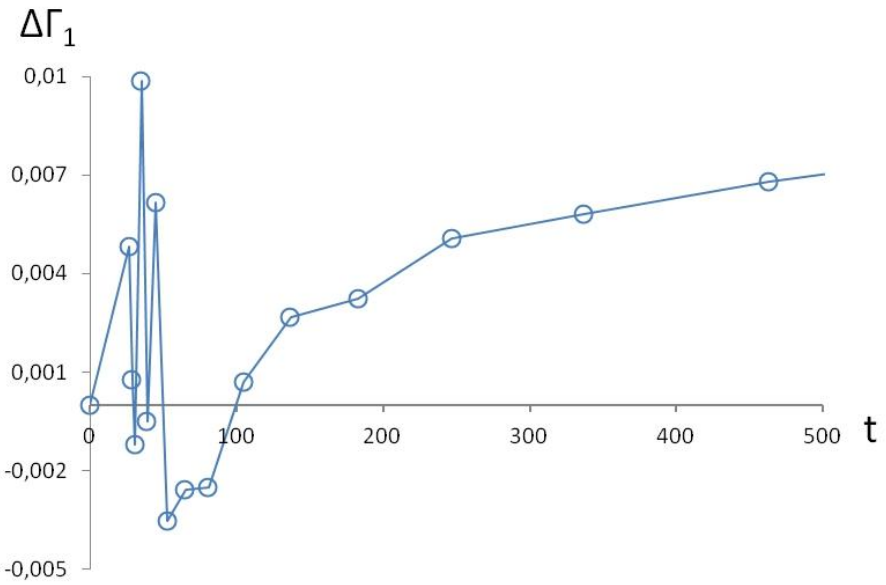

Fig. 2. Variation in absolute error of interface boundary position calculation using nonlinear gradient interpolation with ***erf***-functions compared to the analytical solution.

The absolute error is negligible. For example, for time t = 463 steps, it is $\Delta\Gamma_1$ = 0.006789 (Tabl. 1, Fig. 2). And the relative error does not exceed 0.026 %.

However, the calculation using nonlinear interpolation with ***erf***-functions requires additional calculations at each time step, although it is more accurate compared to other methods proposed earlier.

At the initial moment, the absolute error ΔΓ1 changes sign several times (Fig. 2), in contrast to the behavior of the error ΔΓ when using ordinary two-point schemes for calculating gradients [1]. This indicates that the employed scheme satisfies the conditions of an absolutely stable scheme and the accuracy of the proposed gradient calculation method is of the same order as the accuracy of the concentration field calculations, namely (h^2, τ).

Over time, the absolute error increases slightly. It reaches a maximum (Tabl. 1) at approximately ~ 1000 time steps and then decreases monotonically. This confirms the elimination of the systematic error in the calculation of concentration gradients at the moving phase boundary, as the concentration gradient becomes significantly smoother over time.

The elimination of this accumulating systematic error, which is significant at the beginning of the calculation when the gradients are large, significantly improves the accuracy of the Stefan problem solution. Specifically, we see that the relative error at the time corresponding to 2387 steps is only 0,013 %. In other words, minimizing the systematic error that accumulates over time when solving the Stefan problem using numerical methods with explicit phase boundary tracking improves the computational accuracy by a factor of $n = \frac{\varepsilon_{max}}{\varepsilon} = 10{,}6$.

Conclusions

1. Due to the fact that the actual concentration distribution of the saturating element in all phases of the diffusion coating is a function similar to the ***erf***-function, when calculating concentration gradients at the moving phase boundaries at each time step, an error occurs. This error is systematic and inevitable when solving the Stefan problem using numerical methods with explicit phase boundary tracking. Moreover, these systematic errors in gradient calculation lead to an increase in the velocity of the boundary movement.

2. A method for minimizing the gradient approximation error using nonlinear approximation with the ***erf***-function has been developed, which allows increasing the accuracy of the gradient approximation to the order of (h^2, τ).

3. Calculations have shown that the proposed method has an accuracy of no more than 0,15 %.

4. The elimination of the systematic error significantly increases the accuracy of the Stefan problem solution: the relative error in the calculation of the moving phase boundary coordinate at the end is ε_{max} = 0,0128 %, which is 10,6 times less than in the calculation performed without minimizing the gradient approximation error.

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