NUMERICAL SOLUTION OF THE DIFFUSION PROBLEM IN A TWO-PHASE MEDIUM WITH A MOVING INTERFACE

V. F. Demchenko and S. S. Kozlitina

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Homogeneous difference schemes for numerical solution of the problem of diffusion with a moving interface are constructed on the basis of an integro-interpolation method. The stability and convergence of the schemes are shown. The results of numerical calculation are compared with the analytic solution of the model problem.

The study of diffusion of an impurity in a two-phase medium with a moving interface is closely related to the problem of chemical inhomogeneity in the crystallization of various melts.

Diffusive impurity redistribution is decisive in zone refining of steel and production of semiconductor devices, and appears frequently in fusion welding, crystallization of ingots, and in other metallurgical processes involving crystallization of metals and alloys. Considerable experimental difficulties complicate the quantitative study of unsteady-state diffusion near a crystallization front. Calculation methods that account for the effect of crystallization conditions on the formation mechanism of chemical inhomogeneity are therefore of interest.

There have been a number of works on diffusive impurity redistribution in which an analytic solution is found under certain assumptions (the problem of "diffusive supercooling" in [1], the problem of crystallization of a binary alloy in [2], the problem of chemical inhomogeneity in [3], and others).

In this paper we propose a number of schemes for numerical integration of the one-dimensional problem of chemical inhomogeneity. The formulation of the problem essentially employs the hypothesis of a plane crystallization front.

1. Statement of problem. Mathematically, the process of diffusive impurity redistribution is formulated as a boundary-value problem for parabolic equations with moving discontinuities of the coefficients and special conditions of conjugation at the discontinuity points. The main equations and boundary and initial conditions have the following form:

$$\frac{\partial C_1}{\partial t} = \frac{\partial}{\partial x}\left(D_1 \frac{\partial C_1}{\partial x}\right), \quad 0 < x < \xi(t); \qquad (1)$$

$$\frac{\partial C_2}{\partial t} = \frac{\partial}{\partial x}\left(D_2 \frac{\partial C_2}{\partial x}\right),$$

$$\xi(t) < x < l, \; 0 < t < T; \qquad (2)$$

$$D_1 \frac{\partial C_1}{\partial x}\Big|_{\xi(t)-0} - D_2 \frac{\partial C_2}{\partial x}\Big|_{\xi(t)+0} =$$

$$= \frac{d\xi}{dt}[C_2 - C_1]_{\xi(t)}; \qquad (3)$$

$$C_1|_{\xi(t)-0} = \varkappa C_2|_{\xi(t)+0}; \qquad (4)$$

$$C_1(0, t) = C_1^{(0)}; \quad C_2(l, t) = C_2^{(0)}; \quad C(x, 0) = C_0. \quad (5)$$

Here, C_1 and C_2 are the concentrations of the impurity in the base material; $D_1 = D_1(x, t)$ and $D_2 = D_2(x, t)$ are the diffusion coefficients in phases 1 and 2, respectively; $\xi(t)$ is the position of the interface; and $\varkappa$ is the distribution coefficient (refinement factor). The function $\xi = \xi(t)$ is assumed to be known, and at the initial time $0 < \xi(0) < l$.

In problem (1)–(5) we make the substitution

$$V(x, t) = \begin{cases} C_1(x, t), & 0 \leqslant x \leqslant \xi(t); \\ \varkappa C_2(x, t), & \xi(t) \leqslant x \leqslant l. \end{cases}$$

Then, problem (1)–(5) is transformed as follows:

$$\frac{\partial V}{\partial t} = \frac{\partial}{\partial x}\left(D_1 \frac{\partial V}{\partial x}\right), \quad 0 < x < \xi(t); \qquad (6)$$

$$\frac{1}{\varkappa}\frac{\partial V}{\partial t} = \frac{\partial}{\partial x}\left(\frac{D_2}{\varkappa}\frac{\partial V}{\partial x}\right), \quad \xi(t) < x < l; \qquad (7)$$

$$D_1 \frac{\partial V}{\partial x}\Big|_{\xi(t)-0} - \frac{D_2}{\varkappa}\frac{\partial V}{\partial x}\Big|_{\xi(t)+0} =$$

$$= \frac{d\xi}{dt}\frac{1-\varkappa}{\varkappa} V(\xi(t), t); \qquad (8)$$

$$V(\xi - 0, t) = V(\xi + 0, t); \qquad (9)$$

$$V(0, t) = C_1^{(0)}; \quad V(l, t) = C_2^{(0)}\varkappa;$$

$$V(x, 0) = \begin{cases} C_0(x), & 0 < x < \xi(t), \\ \varkappa C_0(x), & \xi(t) < x < l. \end{cases} \qquad (10)$$

Conjugation condition (8), which relates the flows to the continuous function $V(x, t)$ at the moving interface, can be interpreted as a point (i.e., δ-shaped) power source $d\xi/dt(1 - \varkappa/\varkappa)V(\xi(t), t)\delta(\xi(t) - x)$ ($\delta(z)$ is the Dirac delta function).

The presence of such a source can be taken into account on the right-hand side of the equation, which is understood in the generalized sense:

$$\rho\frac{\partial V}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial V}{\partial x}\right) +$$

$$+ \frac{1-\varkappa}{\varkappa}\frac{d\xi}{dt} V(x, t)\,\delta(\xi(t) - x),$$

$$0<x<l, \qquad (11)$$

where $\rho(x, t)$ and $D(x, t)$ are piecewise-continuous functions, defined as follows:

$$\rho(x, t) = \frac{1}{\varkappa} + \frac{\varkappa - 1}{\varkappa}\eta(\xi(t) - x);$$

$$D(x, t) = \frac{D_2}{\varkappa} + \left(D_1 - \frac{D_2}{\varkappa}\right)\eta(\xi(t) - x);$$

$\eta(\xi(t) - x)$ is the Heaviside unit function:

$$\eta(z) = \begin{cases} 1, & z \geqslant 0, \\ 0, & z < 0. \end{cases}$$

The following equality is valid:

$$\frac{d\xi}{dt} V(x, t)\delta(\xi(t) - x) = \frac{\partial}{\partial t}\left[V(x, t)\eta(\xi(t) - x)\right] - \eta(\xi(t) - x)\frac{\partial V}{\partial t}, \qquad (12)$$

which follows from the relation $\partial[V\eta]/\partial t = (\partial V/\partial t)\eta + V(\partial\eta/\partial t)$, if we take into account that $\partial\eta/\partial t = (\partial\eta/\partial\xi) \times (d\xi/dt) = (d\xi/dt)\delta(\xi(t) - x)$.

We use (12) and transform (11) to

$$\frac{\partial}{\partial t}(\rho V) = \frac{\partial}{\partial x}\left(D\frac{\partial V}{\partial x}\right). \qquad (13)$$

The boundary and initial conditions for $V(x, t)$ are

$$V(0, t) = C_1^{(0)}; \quad V(l, t) = C_2^{(0)}\varkappa;$$

$$V(x, 0) = \begin{cases} C_0(x), & 0 < x < \xi(t), \\ \varkappa C_0(x), & \xi(t) < x < l. \end{cases} \qquad (14)$$

In view of the differentiation of the discontinuous functions ρ and D, problem (13) and (14) is a problem of finding a generalized solution $V(x, t)$.

2. Numerical method. We use the integro-interpolation method of [4] to construct schemes for numerical integration of problem (13) and (14). We partition the interval $[0, l]$ with a network with spacing h, introduce a time step τ such that $x_i = ih$, $t_k = k\tau$ ($i = 1, 2, \ldots, N$; $k = 1, 2, \ldots, K$), and integrate (13) over the elementary region $D_{h\tau}[x_i - h/2 < x < x_i + h/2; t_k \leq t \leq t_{k+1}]$ of the space-time plane (x, t):

$$\int_{t_k}^{t_{k+1}}\int_{x_i-\frac{h}{2}}^{x_i+\frac{h}{2}} \frac{\partial}{\partial t}[\rho V]\,dxdt = \int_{t_k}^{t_{k+1}}\int_{x_i-\frac{h}{2}}^{x_i+\frac{h}{2}} \frac{\partial}{\partial x}\left(D\frac{\partial V}{\partial x}\right)dxdt.$$

We integrate from the left with respect to t and from the right with respect to x:

$$\int_{x_i-\frac{h}{2}}^{x_i+\frac{h}{2}} \left[(\rho V)^{(k+1)} - (\rho V)^{(k)}\right]dx = \int_{t_k}^{t_{k+1}}\left[D\frac{\partial V}{\partial x}\bigg|_{x=x_i+\frac{h}{2}} - D\frac{\partial V}{\partial x}\bigg|_{x=x_i-\frac{h}{2}}\right]dx \qquad (15)$$

(the notation $(\rho V)^{(k+1)}$ indicates the substitution $\rho(x, t_{k+1})V(x, t_{k+1})$).

The integral is calculated from the left by means of the generalized rectangle formula at the midpoint,

$$\int_{x_i-\frac{h}{2}}^{x_i+\frac{h}{2}} (\rho V)^{(k+1)}dx = V_i^{(k+1)}\int_{x_i-\frac{h}{2}}^{x_i+\frac{h}{2}} \rho(x, t_{k+1})dx \quad (V_i^{(k+1)} = V(x_i, t_{k+1})).$$

Several approaches can be used in calculating the integral from the left in (15). We use the method described in [4].

Let $g = D(\partial V/\partial x)$. Then $(\partial V/\partial x) = g/D$ and

$$\int_{x_i}^{x_{i+1}} \frac{\partial V}{\partial x}dx = V(x_{i+1}, t) - V(x_i, t) = \int_{x_i}^{x_{i+1}} \frac{g}{D}dx \approx g\left(x_i + \frac{h}{2}, t\right)\int_{x_i}^{x_{i+1}} \frac{dx}{D(x, t)}.$$

Hence

$$g\left(x_i + \frac{h}{2}, t\right) \approx \frac{V(x_i + h, t) - V(x_i, t)}{h} d_{i+\frac{1}{2}},$$

where

$$d_{i+\frac{1}{2}} = \left[\frac{1}{h}\int_{x_i}^{x_{i+1}} \frac{dx}{D(x, t)}\right]^{-1}.$$

Now we calculate the integral with respect to t using the rectangle formula at the extreme point $t = t_{k+1}$:

$$\int_{t_k}^{t_{k+1}} \left(D\frac{\partial V}{\partial x}\right)_{x_i+\frac{h}{2}} dt \approx \int_{t_k}^{t_{k+1}} \frac{V(x_{i+1}, t) - V(x_i, t)}{h} d_{i+\frac{1}{2}}(t)\,dt = \tau\frac{V_{i+1}^{(k-1)} - V_i^{(k+1)}}{h} d_{i+\frac{1}{2}}^{(k+1)};$$

$$d_{i+\frac{1}{2}}^{(k+1)} = \frac{1}{\tau}\int_{t_k}^{t_{k+1}}\left[\frac{1}{h}\int_{x_i}^{x_{i+1}} \frac{dx}{D(x, t)}\right]^{-1}dt. \qquad (16)$$

Similarly,

$$\int_{t_k}^{t_{k+1}} \left(D\,\frac{\partial V}{\partial x}\right)_{x_i-\frac{h}{2}} dt \approx \tau\,\frac{V_i^{(k+1)} - V_{i-1}^{(k+1)}}{h}\, d_{i-\frac{1}{2}}^{(k+1)}, \quad (17)$$

where

$$d_{i-\frac{1}{2}}^{(k+1)} = \frac{1}{\tau}\int_{t_k}^{t_{k+1}} \left[\frac{1}{h}\int_{x_{i-1}}^{x_i} \frac{dx}{D(x,\ t)}\right]^{-1} dt.$$

We let

$$\rho_i^{(k+1)} = \frac{1}{h}\int_{x_i-\frac{h}{2}}^{x_i+\frac{h}{2}} \rho(x,\ t_{k+1})\,dx,$$

$$\rho_i^{(k)} = \frac{1}{h}\int_{x_i-\frac{h}{2}}^{x_i+\frac{h}{2}} \rho(x,\ t_k)\,dx \quad (18)$$

and substitute into (15) the obtained expressions for the integrals in terms of the finite sums:

$$\frac{\rho_i^{(k+1)} v_i^{(k+1)} - \rho_i^{(k)} v_i^{(k)}}{\tau} =$$

$$= \frac{1}{h^2}\left[d_{i+\frac{1}{2}}^{(k+1)} \left(v_{i+1}^{(k+1)} - v_i^{(k+1)}\right) - d_{i-\frac{1}{2}}^{(k+1)} \left(v_i^{(k+1)} - v_{i-1}^{(k+1)}\right) \right],$$

$$i = 1,\ 2,\ \ldots,\ N-1. \quad (19)$$

System of difference equations (19), whose coefficients are found from formulas (16)–(18), defines a calculation scheme (scheme I) for the network function $v_i^{(k+1)}$ ($i = 1, 2, \ldots, N-1$; $k = 1, 2, \ldots, K$).

Some modifications of this scheme are possible.

We integrate the expression for the flow $g = D(\partial V/\partial x)$ with respect to x from x_i to x_{i+1}

$$\frac{1}{h}\int_{x_i}^{x_{i+1}} g(x,\ t)\,dx = \frac{1}{h}\int_{x_i}^{x_{i+1}} D\,\frac{\partial V}{\partial x}\,dx. \quad (20)$$

We approximate the integrals in (20) as follows:

$$\frac{1}{h}\int_{x_i}^{x_{i+1}} g(x,\ t)\,dx \approx g\left(x_i + \frac{h}{2},\ t\right);$$

$$\frac{1}{h}\int_{x_i}^{x_{i+1}} D\,\frac{\partial V}{\partial x}\,dx \approx \left.\frac{\partial V}{\partial x}\right|_{x_i+\frac{h}{2}} \frac{1}{h}\int_{x_i}^{x_{i+1}} D(x,\ t)\,dx \approx$$

$$\approx \frac{V(x_{i+1},\ t) - V(x_i,\ t)}{h}\, d_{i+\frac{1}{2}}(t);$$

$$d_{i+\frac{1}{2}}(t) = \frac{1}{h}\int_{x_i}^{x_{i+1}} D(x,\ t)\,dx.$$

Hence

$$g\left(x_{i+\frac{1}{2}},\ t\right) \approx \frac{V(x_{i+1},\ t) - V(x_i,\ t)}{h}\, d_{i+\frac{1}{2}}(t); \quad (21)$$

Similarly,

$$g\left(x_{i-\frac{1}{2}},\ t\right) \approx \frac{V(x_i,\ t) - V(x_{i-1},\ t)}{h}\, d_{i-\frac{1}{2}}(t), \quad (22)$$

where

$$d_{i-\frac{1}{2}}(t) = \frac{1}{h}\int_{x_{i-1}}^{x_i} D(x,\ t)\,dx.$$

We replace in (15) the flows at points $x_i + h/2$ and $x_i - h/2$ by their approximate values from (21) and (22) and integrate with respect to t just as for scheme I. Then the formulas for the coefficients $d_{i+\frac{1}{2}}^{(k+1)}$ and $d_{i-\frac{1}{2}}^{(k+1)}$ in difference equation (19) will have the following form:

$$d_{i+\frac{1}{2}}^{(k+1)} = \frac{1}{\tau}\int_{t_k}^{t_{k+1}} d_{i+\frac{1}{2}}(t)\,dt;$$

$$d_{i-\frac{1}{2}}^{(k+1)} = \frac{1}{\tau}\int_{t_k}^{t_{k+1}} d_{i-\frac{1}{2}}(t)\,dt. \quad (23)$$

The difference scheme for Eq. (19) in which the coefficients are calculated by (18) and (23) we call difference scheme II. Note that in a number of cases scheme II coincides with the scheme obtained by preliminary smoothing of the discontinuous coefficients in (13) and subsequent replacement of the derivatives in the equation with smooth coefficients by their difference ratios.

The error of approximation of differential equation (13) by finite-difference equation (19) can be obtained if certain assumptions are made about the properties of the solution V(x, t) up to the discontinuity limit of the coefficients. For this, the remainder terms in the formulas for numerical integration and differentiation should be estimated. If the elementary region $D_{h\tau}$

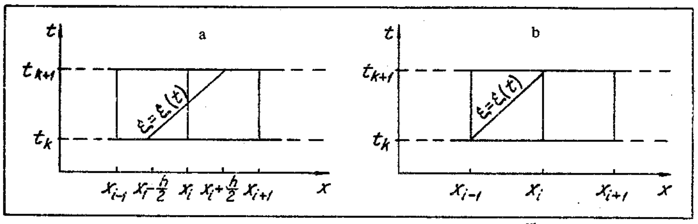

Fig. 1. Fragments of space-time network.

does not contain the line $\xi(t)$, then the approximation error of schemes I and II is $O(\tau + h^2)$. In the vicinity of points $x = \xi(t)$, the order of approximation of the differential equation deteriorates and is a function of the way in which the boundary $\xi(t)$ intersects the lines of the space-time network.

Let us consider a few simple cases of such intersections and derive formulas for the coefficients in difference equation (19) for schemes I and II.

Let the time step τ be such that the boundary $\xi(t)$ moves in time τ exactly one step of the space network, being at all times exactly in the middle between the nodes of the network. A fragment of a space-time network corresponding to this case is shown in Fig. 1a ($d\xi/dt > 0$).

We assume that the function $\xi(t)$ can be approximated with sufficient accuracy by a polygonal function that coincides with $\xi(t)$ at points $t = t_k$ ($k = 1, 2, \ldots, K$) and is linear between them. Let us consider the case of piecewise-constant coefficients:

$$D = \begin{cases} D_1 = \text{const}, & 0 < x < \xi(t), \\ D_2 = \text{const}, & \xi(t) < x < l. \end{cases}$$

Then the coefficients of the difference equation are easily calculated and have the form:

for scheme I

$$\rho_i^{(k+1)} = 1, \quad \rho_i^{(k)} = \frac{1}{\varkappa};$$

$$d_{i+\frac{1}{2}}^{(k+1)} = \frac{D_2}{2} + \frac{D_1 D_2}{D_2 - D_1} \ln \frac{D_1 + D_2}{2D_1};$$

$$d_{i-\frac{1}{2}}^{(k+1)} = \frac{D_1}{2} + \frac{D_1 D_2}{D_2 - D_1} \ln \frac{2D_2}{D_2 + D_1}; \tag{24}$$

for scheme II

$$\rho_i^{(k+1)} = 1, \quad \rho_i^{(k)} = \frac{1}{\varkappa};$$

$$d_{i+\frac{1}{2}}^{(k+1)} = \frac{D_1 + 7D_2}{8}; \quad d_{i-\frac{1}{2}}^{(k+1)} = \frac{7D_1 + D_2}{8}. \tag{25}$$

If the line $\xi = \xi(t)$ intersects the network as shown in Fig. 1b, the coefficients of the difference equation have the form:

for scheme I

$$\rho_i^{(k+1)} = 1, \quad \rho_i^{(k)} = \frac{\varkappa + 1}{2\varkappa};$$

$$d_{i-\frac{1}{2}}^{(k+1)} = D_1, \quad d_{i+\frac{1}{2}}^{(k+1)} = \frac{D_1 D_2}{D_2 - D_1} \ln \frac{D_2}{D_1}; \tag{26}$$

for scheme II

$$\rho_i^{(k+1)} = 1, \quad \rho_i^{(k)} = \frac{\varkappa + 1}{2\varkappa};$$

$$d_{i+\frac{1}{2}}^{(k+1)} = \frac{D_1 + D_2}{2}; \quad d_{i-\frac{1}{2}}^{(k+1)} = D_1. \tag{27}$$

3. Stability of numerical integration schemes. Let $z_i^{(k+1)} = V_i^{(k+1)} - v_i^{(k+1)}$ be the error of the method of numerical solution ($V_i^{(k+1)} = V(x_i, t_{k+1})$). We substitute $v_i^{(k+1)} = -V_i^{(k+1)} + z_i^{(k+1)}$ into (19) and obtain for $z_i^{(k+1)}$ a difference boundary-value problem:

$$\frac{\rho_i^{(k+1)} z_i^{(k+1)} - \rho_i^{(k)} z_i^{(k)}}{\tau} = \frac{1}{h^2}\Big[d_{i+\frac{1}{2}}^{(k+1)} (z_{i+1}^{(k+1)} - z_i^{(k+1)}) - d_{i-\frac{1}{2}}^{(k+1)} (z_i^{(k+1)} - z_{i-1}^{(k+1)}) \Big] + \psi_i^{(k+1)},$$

$$i = 1, 2, \ldots, N-1; \quad z_0^{(k+1)} = 0; \quad z_N^{(k+1)} = 0, \tag{28}$$

where

$$\psi_i^{(k+1)} = \frac{1}{h\tau}\Bigg\{ \int_{x_i - \frac{h}{2}}^{x_i + \frac{h}{2}} [(\rho V)^{(k+1)} - (\rho V)^{(k)}]\, dx - \int_{t_k}^{t_{k+1}} \Big[D\frac{\partial V}{\partial x}\Big|_{x_i + \frac{h}{2}} - D\frac{\partial V}{\partial x}\Big|_{x_i - \frac{h}{2}} \Big] dt \Bigg\} - \frac{\rho_i^{(k+1)} v_i^{(k+1)} - \rho_i^{(k)} v_i^{(k)}}{\tau} + \frac{1}{h^2}\Big[d_{i+\frac{1}{2}}^{(k+1)} (v_{i+1}^{(k+1)} - v_i^{(k+1)}) - d_{i-\frac{1}{2}}^{(k+1)} (v_i^{(k+1)} - v_{i-1}^{(k+1)}) \Big]$$

is the order of approximation of the differential equation by the difference equation.

Let us rewrite (28) as

$$a_i^{(k+1)} z_{i+1}^{(k+1)} - b_i^{(k+1)} z_i^{(k+1)} + c_i^{(k+1)} z_{i-1}^{(k+1)} = f_i^{(k+1)}$$

$$(i = 1, 2, \ldots, N-1), \tag{29}$$

where

$$a_i^{(k+1)} = \frac{d_{i+\frac{1}{2}}^{(k+1)} \tau}{h^2 \rho_i^{(k+1)}}; \quad c_i^{(k+1)} = \frac{d_{i-\frac{1}{2}}^{(k+1)} \tau}{h^2 \rho_i^{(k+1)}};$$

$$b_i^{(k+1)} = a_i^{(k+1)} + c_i^{(k+1)} + 1;$$

$$f_i^{(k+1)} = -\psi_i^{(k+1)} \tau - \frac{\rho_i^{(k)}}{\rho_i^{(k+1)}} z_i^{(k)}.$$

For second-order difference equations such as (29) with boundary conditions $z_0^{(k+1)} = z_N^{(k+1)} = 0$, we have the maximum principle [5]

$$\max_i |z_i^{(k+1)}| \leqslant \frac{1}{\delta} \max_i |f_i^{(k+1)}|, \tag{30}$$

if the coefficients of the difference equation satisfy the conditions

$$a_i^{(k+1)} > 0, \qquad c_i^{(k+1)} > 0,$$

$$b_i^{(k+1)} \geqslant a_i^{(k+1)} + c_i^{(k+1)} + \delta^{(k+1)}, \qquad \delta^{(k+1)} > 0.$$

We introduce the norms for the vectors as follows: $\|y\| = \max_i |y_i|$. Then (30) can be rewritten as

$$\|z^{(k+1)}\| \leqslant \|f^{(k+1)}\| \leqslant \|\psi^{(k+1)}\| \frac{\tau}{\delta^{(k+1)}} + p^{(k+1)} \|z^{(k)}\|, \tag{31}$$

where

$$\delta^{(k+1)} = \min_i \rho_i^{(k+1)}, \quad p^{(k+1)} = \max_i \frac{\rho_i^{(k)}}{\rho_i^{(k+1)}}.$$

Theorem. Difference scheme (19) is uniformly stable for initial data.

From (31), by recurrent substitution for $\|z^{(k+1)}\|$, $\|z^{(k-1)}\|, \ldots$ we obtain

$$\|z^{(k+1)}\| \leqslant \tau \left(\frac{\|\psi^{(k+1)}\|}{\delta^{(k+1)}} + \frac{p^{(k+1)}}{\delta^{(k)}} \|\psi^{(k)}\| + \cdots \right.$$

$$\left. \cdots + \frac{p^{(k+1)} p^{(k)} \ldots p^{(2)}}{\delta^{(1)}} \|\psi^{(k)}\| \right) +$$

$$+ p^{(k+1)} p^{(k)} \ldots p^{(1)} \|z^{(0)}\| \leqslant \frac{\tau}{\delta_\tau} \|\psi\|_\tau \sum_{j=0}^{k} p_\tau^j +$$

$$+ p_\tau^{k+1} \|z^{(0)}\|.$$

Here $p_\tau = \max_k p^{(k)}$, $\delta_\tau = \min_k \delta^{(k)}$, $\|\psi\|_\tau = \max_k \|\psi^{(k)}\|$.

We represent p_τ as $p_\tau = 1 + R\tau$, where R is an arbitrary constant that is consistent with the inequality $p_\tau > 0$. Then from

$$\|z^{(k+1)}\| \leqslant \frac{e^{RT} - 1}{R\,\delta_\tau} \|\psi\|_\tau + e^{RT} \|z^{(0)}\| =$$

$$= M_1 \|\psi\|_\tau + M_2 \|z^{(0)}\| \qquad (32)$$

follows the uniform stability of difference scheme (19) for initial data.

In the particular case of R = 0, estimate (32) is valid, since $\lim_{R \to 0} \frac{e^{RT} - 1}{R} = T$. The convergence of the solution of the difference problem on the solution of the differential problem at a rate equal to the order of approximation also follows from (32).

4. Numerical experiments. In order to check these schemes, the numerical solution was compared with the analytic solution obtained in [3] for an infinite rod, a constant velocity of the phase boundary, and equal diffusion coefficients. The model problem was calculated with the following parameters:

$$C_1^{(0)} = C_2^{(0)} = C_0 = 0{,}04; \ \varkappa = 0{,}05; \ D_1 = 10^{-5},$$

$$D_2 = 10^{-5}; \ h = 10^{-5}; \ \tau = 10^{-3}; \ \frac{d\xi}{dt} = 10^{-2},$$

and the length of the interval $[0, l]$ was such that the boundary conditions had practically no effect in the numerical solution.

Figure 2 shows the results of calculation of the model problem by the method proposed in Section 2 (using formula (26)) and of the analytic solution [3]. The table gives the exact and calculated values for time t = 0.04 sec.

The examples show that the difference schemes can be used for diffusion problems with a moving phase boundary. In developing the schemes described here, we also tried six-point schemes and schemes based on

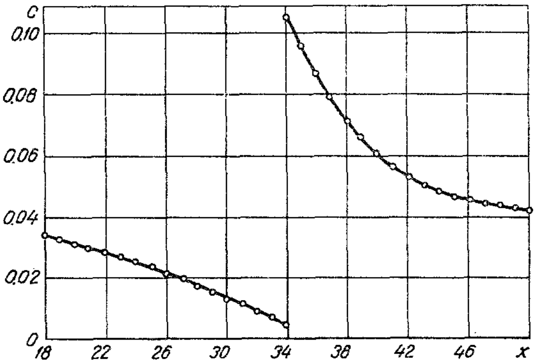

Fig. 2. Distribution of impurity concentration (solid line, exact solution; points, numerical calculation; C in %; x in μ).

Exact and Calculated Values for Time t = 0.04 sec

x; μ	Exact values	Calculated solutions		
		by (24)	by (26)	by (25)
2	0.029121	0.029478	0.029241	0.029385
4	0.025510	0.025907	0.025637	0.025798
6	0.021453	0.021857	0.021567	0.021736
8	0.017151	0.017526	0.017337	0.017399
10	0.012860	0.013176	0.012910	0.013050
12	0.008851	0.009093	0.008874	0.008977
14	0.005374	0.005541	0.005334	0.005441
16	0.087006	0.087920	0.086517	0.088167
18	0.071886	0.072637	0.071621	0.072827
20	0.061007	0.061616	0.060902	0.061760
22	0.053407	0.053900	0.053413	0.054004

various kinds of smoothing of discontinuous coefficients. In the numerical experiments, the six-point scheme had some instability (sawtooth solution). The schemes with smoothing gave satisfactory solutions for small smoothing intervals—one or two steps of the network.

The proposed procedure can be extended to the multidimensional case (the authors have solved the two-dimensional problem), and also to more general equations and systems of equations for solving the problem of thermal diffusion.

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Paton Institute of Electric Welding, Kiev