In conclusion, let us note that the method proposed can be modified. Thus, if the outer given temperature varies sufficiently smoothly during a long time, then there is every foundation to consider that the relationship (19) remains valid in this interval. The problem can then be solved by partitioning τ into a number of finer sections which will be the computation steps, and the value of the temperature, obtained in the previous interval, just for the value $\tau = 1$, will be used when going over to the next value of h_m^j. In the case mentioned, such an approach is more efficient.

NOTATION

t	is the time;
z	is the coordinate;
$T(z, t)$	is the temperature;
$\lambda(z, t)$, $a(z, t)$	are the coefficients of thermal conductivity and thermal diffusivity, respectively;
$h_m(t)$	are the coordinates of the phase-interface position;
H	is the lower boundary coordinate;
L	is the heat of the phase transition;
γ	is the volume weight of the soil;
$w^0(z)$	is the given moisture distribution in the soil;
w_0	is the experimentally determined quality of moisture which does not freeze at 0°C.

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SEMI-ANALYTICAL ALGORITHM FOR THE APPROXIMATE SOLUTION OF A NONSTATIONARY INVERSE PROBLEM OF DIFFUSION ON THE BASIS OF A DIRECT METHOD OF SOLUTION, LINEAR PROGRAMMING, AND REGULARIZATION METHODS

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Some analytical solutions of the direct problem of diffusion are presented for infinite bodies. The direct solutions constructed are used in algorithms for the approximate solution of the nonstationary inverse diffusion problem.

Results directly concerning the process of diffusion scattering of a substance are elucidated below. However, because of the analogy between the thermal conduction and diffusion processes, the results obtained are automatically carried over to the contiguous thermal-conductivity problem.

Let $0\xi\eta\zeta$ and $0xyz$ be the combined Cartesian reference systems with the ζ and z axes directed downward.

Let us consider the free diffusion process in a half-space (in the absence of sources and sinks):

$$V = \{(\xi, \eta, \zeta): |\xi| < \infty, |\eta| < \infty, \zeta \geqslant 0\}. \quad (1)$$

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At the time $\tau = \tau_0$ preceding the beginning of the process of diffusion scattering of a substance in V, the concentration distribution C_0 of the substance is independent of ζ and subject to the law $C_0 = F(\xi, \eta)$. There is no mixing of the substance in the vertical direction. The diffusion, which initially encloses the horizon $\zeta = 0$ and is propagated into the depths with time, will proceed on each of the horizons $\zeta = h$ with its constant diffusion coefficient $D^{(h)}$, so that for the whole half-space V

$$D = D(\zeta, \tau) = \begin{cases} 0, & \tau < \tau^{(h)} \\ D^{(h)}, & \tau \geqslant \tau^{(h)} \end{cases}, \quad \zeta = h \in [0, \infty). \tag{2}$$

Here $\tau^{(h)}$ is the time at which the diffusion process reaches the horizon $\zeta = h$, where $\tau^{(0)} = \tau_0$.

The process described is characteristic to the formation of diffusion aureoles, developed on planar and slightly convex slopes under rare and nonferrous metal deposits. The aureoles mentioned originate by means of chaotic displacement (free diffusion) into the enclosing waste rock material formed from the upper horizons of the bedrock because of the effect of different surface physical reagents thereon [1, 2].

Interpretation of the aureoles, which consists of predicting the distribution $C_0(\xi)$ of some chemical element in early deep bedrock according to known estimates of its distribution C(x) in the aureole and of separate values of $C^{(i)}$ of the desired function $C_0(\xi)$ (known from the results of assaying outcrops), reduces in the one-dimensional case $F = F(\xi)$ to solving the integral equation

$$C(x, \sigma) = \frac{1}{\sqrt{2\pi}\,\sigma} \int_{-\infty}^{\infty} C_0(\xi) \exp\left[-\frac{(x-\xi)^2}{2\sigma^2}\right] d\xi \tag{3}$$

under the conditions

$$C_0(\xi_i) = C^{(i)}, \quad \xi_i \in (-\infty, \infty), \quad i = \overline{0, n}. \tag{4}$$

Hence, the diffusion scattering parameter $\sigma = \sqrt{2D\tau}$ is an unknown quantity.

Let us note that in practice it is not required to obtain the solution on the whole axis but only in some interval (α, β).

The problem (3)-(4) is of definite theoretical interest, since the majority of developments are devoted to inverse boundary-value problems [3-6], while algorithms to determine the coefficients of the diffusion (heat conduction) equation, just like the preceding concentration and temperature distributions over their running fields, have as yet been studied in less detail. We limit ourselves to the case of giving the quantity $C_0(\xi)$ at one point:

$$C_0(\xi_0) = C^{(0)}, \quad \xi_0 \in (-\infty, \infty). \tag{5}$$

Let us first consider the solution of the direct problem (3) for fixed σ. An analytical method for seeking $C(x, \sigma)$ approximately is given in [7], based on a polynomial approximation of the field $C_0(\xi)$:

$$C_0(\xi) = \sum_{i=0}^{L} A_i \psi_i^{(1)}(\xi), \quad \psi_i^{(1)} \in \Psi^{(1)} = \{\xi^i\}_{i=0}^{\infty}. \tag{6}$$

Let us mention the two model classes $\Psi^{(2)}$ and $\Psi^{(3)}$ of functions which are sufficiently convenient for the approximation of continuous and piecewise-continuous distributions and which admit of solvability of the right side of (3) in elementary functions:

$$\Psi^{(2)} = \{1, \{\sin i\xi\}_{i\in N^-}, \{\cos i\xi\}_{i\in N^+}\},$$
$$N^- = \{2m-1\}_1^{\infty}, \quad N^+ = \{2m\}_1^{\infty}, \tag{7}$$
$$\Psi^{(3)} = \{\exp(-i\xi)\}_{i=0}^{\infty}. \tag{8}$$

Let $\bar{\Psi}^{(2)}$ and $\bar{\Psi}^{(3)}$ denote the spaces of all possible linear combinations of the functions $\psi_i^{(2)}$ and $\psi_i^{(3)}$ from the classes $\Psi^{(2)}$ and $\Psi^{(3)}$, with real coefficients.

It is known that the class of functions $\Psi^{(2)}$ is closed in the space $L_2(0, 2\pi)$ of square integrable functions, while the class $\Psi^{(3)}$ is closed in the space $L_2(0, \infty)$ with the weight function $\exp(-\xi)$ [8]. Let us note that the segment (α, β) being studied can always be included in the interval $(0, \infty)$ or $(0, 2\pi)$ by a linear transformation.

The expediency of introducing each new universal class $\Psi^{(k)}$ is dictated by practical requirements in high-speed algorithms: The presence of a wide set of classes $\Psi^{(k)}$ permits a significant reduction in the number L of terms in the approximating construction (6) for a given degree of approximation both because of the selection of the class $\Psi^{(k)}$ of functions closest to the approximation and because of the combination of functions ψ_i^k of different classes $\Psi^{(k)}$.

According to [9], the solution of the direct problem in the spaces $\overline{\Psi}^{(2)}$ and $\overline{\Psi}^{(3)}$ is given by the following formulas:

$$C(x, \sigma) = \frac{1}{\sqrt{2\pi}\,\sigma} \int_{-\infty}^{\infty} \left[A_0 + \sum_{i=1}^{L} (A_{2i-1} \sin i\xi + A_{2i} \cos i\xi)\right] \times$$

$$\times \exp\left[-\frac{(x-\xi)^2}{2\sigma^2}\right] d\xi = A_0 + \sum_{i=1}^{L} (A_{2i-1} \sin ix + A_{2i} \cos ix) \exp[-(i\sigma)^2/2], \tag{9}$$

$$C(x, \sigma) = \frac{1}{\sqrt{2\pi}\,\sigma} \int_{-\infty}^{\infty} \left[\sum_{i=0}^{L} A_i \exp(-i\xi)\right] \exp\left[-\frac{(x-\xi)^2}{2\sigma^2}\right] d\xi = \sum_{i=0}^{L} A_i \exp[(i\sigma)^2/2] \exp(-ix). \tag{10}$$

The transformation (3) transforms the spaces $\overline{\Psi}^{(2)}$ and $\overline{\Psi}^{(3)}$ into themselves.

We obtain the approximate solution of the direct problem for the arbitrary function by expanding it (for an L selected a priori) in the components $\sin i\xi$, $\cos i\xi$ [or $\exp(-i\xi)$]. The coefficients of these expansions participate directly, according to (9) and (10), in the formation of the approximating functions C(x) from the model spaces $\overline{\Psi}^{(2)}$ and $\overline{\Psi}^{(3)}$.

Let us note that the approximation approach to solving the direct and inverse problems of heat conduction was practiced earlier, in the papers [4, 10, 11] for instance.

Let us investigate the problem of solvability of the problem (3)-(5).

1. We find first that for fixed σ the solution of (3) is unique. Upon imposition of bilateral constraints on the variation of $C_0(\xi)$ (this should be dictated by the physical crux of the problem) the inverted problem (3) meanwhile becomes correctly formulated [12].

2. For unknown σ and no constraints (5), Eq. (3) has a nondenumerable set of solutions.

Two different distributions –

$$C_0^{(1)}(\xi) = A_0^{(1)} + \sum_{i=1}^{L_1} (A_{2i-1}^{(1)} \sin i\xi + A_{2i}^{(1)} \cos i\xi),$$

$$C_0^{(2)}(\xi) = A_0^{(2)} + \sum_{i=1}^{L_2} (A_{2i-1}^{(2)} \sin i\xi + A_{2i}^{(2)} \cos i\xi) \quad (L_1 > L_2)$$

– are transformed by using the integral transform (3) into the same function $C(x) \in \overline{\Psi}^{(2)}$ if and only if

$$A_i^{(1)} \exp[-(i\sigma_1)^2/2] = A_i^{(2)} \exp[-(i\sigma_2)^2/2], \qquad A_j^{(1)} \equiv 0, \quad i = \overline{0, L_2}, \quad j = \overline{L_2+1, L_1}. \tag{11}$$

The function $C(x) \in \overline{\Psi}^{(3)}$ is the mapping of the two distributions

$$C_0^{(1)}(\xi) = \sum_{i=0}^{L_1} A_i^{(1)} \exp(-i\xi), \quad C_0^{(2)}(\xi) = \sum_{i=0}^{L_2} A_i^{(2)} \exp(-i\xi) \quad (L_2 < L_1)$$

only in the case

$$A_i^{(1)} \exp[(i\sigma_1)^2/2] = A_i^{(2)} \exp[(i\sigma_2)^2/2], \qquad A_j^{(1)} \equiv 0, \quad i = \overline{0, L_2}, \quad j = \overline{L_2+1, L_1}. \tag{12}$$

The relations (11) and (12) determine a nondenumerable set of solutions of the inverse problem (3) in the spaces $\Psi^{(2)}$ and $\Psi^{(3)}$.

3. Now let the inverse problem (3) be solved in $\overline{\Psi}^{(2)}$ and $\overline{\Psi}^{(3)}$ under the constraints (5). Without limiting the generality, let us consider the value of L to be known. Let us consider the class $\Psi^{(3)}$. Having been given an arbitrary value of $\sigma = \sigma_0$, let us expand the function $C(x, \sigma_0)$ in the components $\varphi_i^{(3)}(x) = \exp[(i\sigma_0)^2/2]\exp(-ix)$ (i =

0, L) (without a remainder), and let us thereby determine the unique solution $C_0(\xi, \sigma_0)$ of (3) for fixed σ. In the general case the curve $C_0(\xi, \sigma_0)$ does not pass through the point $(\xi_0, C^{(0)})$ and therefore does not belong to the set $\{C_0^{(t)}(\xi, \sigma_t), \{B_i(\sigma_t)\}_{i=\overline{0,L}}\}_{t\in T}$ of the solutions of problem (3)-(5), whose number is denoted by the subscript t, running through the subscript set T; the coefficients are denoted as B_i.

The following equality holds:

$$\sum_{i=0}^{L} \exp(-i\xi_0)[B_i(\sigma_t) - A_i(\sigma_0)] + C_0(\xi_0, \sigma_0) - C^{(0)} = 0. \tag{13}$$

By means of (12), let us express the unknown B_i in (13) in terms of the desired σ_t and the known A_i and σ_0; hence, we obtain an equation for σ_t

$$\sum_{i=0}^{L} A_i(\sigma_0)\exp(-i\xi_0)\left\{\exp\left[\frac{i^2(\sigma_0^2-\sigma_t^2)}{2}\right]-1\right\} + C_0(\xi_0, \sigma_0) - C^{(0)} = 0. \tag{14}$$

Using the notation

$$K_0 = -\sum_{i=0}^{L} A_i(\sigma_0)\exp(-i\xi_0) + C_0(\xi_0, \sigma_0) - C^{(0)}, \tag{15}$$

$$K_i = A_i(\sigma_0)\exp(-i\xi_0)\exp((i\sigma_0)^2/2) \quad (i = \overline{1, L}), \tag{16}$$

we arrive at the algebraic equation

$$\sum_{i=0}^{L} K_i y^{i^2} = 0, \quad y = \exp(-\sigma_t^2/2). \tag{17}$$

Let us determine its roots; they will not be greater than L^2. Let us extract the real roots which satisfy the condition $0 < y \le 1$. Let these be $y_1, y_2, \ldots, y_s$; $s \le L^2$. Then the desired σ_t are defined as $\sigma_t = \sqrt{-2\ln y_t} \ge 0$, $t = \overline{1, s}$. Substituting the values found for σ_t in the relationship (12), we obtain all the s of the equally possible formal solutions of the problem (3)-(5).

Therefore, knowledge of the magnitude of the desired function $C_0(\xi)$ at a single point ξ_0 still does not free the solution of the problem (3)-(5) from uncertainty; however, giving condition (5) in a cardinal manner reduces the spectrum of the solutions of (3) by permitting the extraction of a finite number of them (perhaps just one) from the nondenumerable set of the latter. Excluding the physically inadmissible solutions for the s solutions found, the scope of the uncertainty of the solution can be narrowed still more.

Analogous deductions are also valid for the space $\overline{\Psi}^{(2)}$.

4. The giving of L^2 constraints (5) at any points ξ_i makes the solution of the problem completely unique. Moreover, it is clear that uniqueness of the solution of (3) can be achieved by assuming, in addition to the value $C^{(0)}$ given a priori, still another value $C^{(1)}$ of the function $C_0(\xi)$ but a posteriori of the given point ξ_1.

Now let us construct an algorithm for the approximate solution of the problem (3)-(5). Let us agree to denote the true distribution by C(x) as before and the observed and approximate distributions, respectively, by $\tilde{C}(x)$ and $C^*(x)$.

Let us consider the direct method of solution based on inversion of (9) and (10). Given a sufficiently large L and the value $\sigma = \sigma_0 = 1$, let us approximate the function $\tilde{C}(x)$ by the model $C^*(x, \sigma_0)$ from the space $\overline{\Psi}^{(2)}$ or $\overline{\Psi}^{(3)}$. Using the solution $C_0^*(\xi)$ found and assuming the value $C^{(0)}$, we determine all s formal solutions of the problem (3)-(5) by the algorithm described above, and we then extract a finite number N of the physically acceptable, equally probable, possible solutions in the absence of additional information.

Since the real class of possible distributions $C_0(\xi)$ is considerably broader than the model classes, the method described should refer to algorithms of the solution to inverse problems within the framework of a selection method permitting a search for at least one solution of the problem. Let us note that the model class may not contain an acceptable solution of the problem (3)-(5) in addition to the case $s > 1$.

Comparing the proposed semianalytical method with direct numerical methods, we can state the following.

1. Annihilation of the need to replace the initial operator by a finite algebraic sum, as the predominant majority of numerical algorithms require, raises the stability of the solution to the calculation process.

2. To achieve the required accuracy of the approximation, the model function $C_0^*(\xi)$, for which the number of free parameters is considerably less than the number of points of the discrete function needed to assure the same degree of approximation, can be used.

3. In the case of a strongly oscillating C(x) when a larger L is formally required because of the smoothness of the model functions, it is nevertheless possible to get used to a considerably smaller L, since sections of the pulse character for the change in $C_0(\xi)$, which are due to local inhomogeneities of the medium, are sometimes not of interest for practical purposes and are subject to smoothing.

By virtue of the Hadamard incorrectness of the problem (3)-(5), an increase in the number L of parameters $C_0^*(\xi)$ in the interests of assuring a more detailed description of $C_0(\xi)$ inevitably results in instability of the unregularized solution resulting from the physical crux of the problem itself. However, in definite cases [low interference level in $\tilde{C}_{(x)}$, a dense recording mesh for values of C(x), low value of L] the requirement for such solutions to obtain rough express-information is completely legitimate. The authors of [5, 11] arrived at a similar deduction relative to the solution in boundary-value problems.

Now, besides (5), let it be known that the curve $C_0(\xi)$ is included in the interval (C_{min}, C_{max}) in $[\alpha, \beta]$; rough majorant boundaries for C_{min} and C_{max} can always be indicated by starting from physical considerations: $C_{min} \leq C_0(\xi) \leq C_{max}$, $\xi \in [\alpha, \beta]$. Let us also assume the errors in the values $\tilde{C}(x)$ do not exceed some given $\delta > 0$: $\|\tilde{C}(x) - C(x)\| \leq \delta$ in the norm: [for definiteness, we take the maximum deviation of $\tilde{C}(x)$ from C(x) as the norm]. Here it is convenient to carry out the solution on the basis of functional programming methods.

Let us initially construct an algorithm for fixed σ. It is required to solve the following generalized linear programming problem:

$$\max_{j=\overline{1,n}} |C^*(x_j) - \tilde{C}(x_j)| = \min_{A_i} \tag{18}$$

for a constraint in the form of the equality

$$\sum_{i=0}^{L} A_i \psi_i^{(k)}(\xi_0) = C^{(0)} \tag{19}$$

and a nondenumerable set of constraints of the form of the inequalities

$$C_{\min} \leqslant \sum_{i=0}^{L} A_i \psi_i^{(k)}(\xi) \leqslant C_{\max}, \quad \xi \in [\alpha, \beta], \tag{20}$$

where n is the number of points recording the field $\tilde{C}(x)$, and the structure of the function $C^*(x)$ is defined by the right side of (9) or (10).

Formulation of the problem (18)-(20) in a known manner reduces to a standard [13], and by virtue of the compactness of the domain of variation of the coefficients $\psi_i^{(k)}$ for the desired A_i in (20) it can be solved by the inverse matrix method [14].

Since L plays the part of a natural regularization parameter [6], in order to raise the stability of the solution it is necessary to select the least possible $L = L_0$ admitting solvability of the problem (18)-(20) under the condition

$$|C^*(x) - \tilde{C}(x)| \leqslant \delta. \tag{21}$$

We find the lower bound L_{min} for L_0 by means of the absolute minimization of the functional (18) for values of L starting with 0 and growing successively by one [in other words, by clarifying the compatibility of the system of n two-sided inequalities of the type (21)]. Then the first minimum L for which the functional does not exceed δ is indeed L_{min} with which the solution of the problem (18), (19), (20) must start and the growth of L must continue in the case of no assurance as to compliance with condition (21).

A simpler algorithm for the solution of the problem with fixed σ can be indicated, for which we cover $[\alpha, \beta]$ by a mesh $\{\xi_i\}_{i=1}^{m}$ and we demand compliance with condition (20) only at its nodes. Replacement of the nondenumerable set of constraints by a finite number results in the classical linear programming problem, whose known methods of solution [15] are sufficiently simpler than the inverse matrix method. Although weakening of the constraints (20) can drive the curve $C_0^*(\xi)$ beyond admissible limits, it is completely competent in definite cases, since the boundaries of C_{min} and C_{max} are usually known to the error ρ, and the field $C_0^*(\xi)$ can be enclosed in the interval ($C_{min} - \rho$, $C_{max} + \rho$) by compressing the grid. Moreover, it is sometimes required to obtain only a qualitative solution, i.e., to clarify the pole of condensation of the concentration without its quantitative estimation.

If σ is desired, the solution of the problem can be obtained by varying σ in a mesh of values $\Sigma = \{\sigma_k\}$ given in some reasonable limits and by using the solution of the algorithm for fixed σ in each cycle. We select σ_k as desired, for which the solution is achieved for least L. After the construction of such a $C_0^*(\xi)$, the possible solutions of the problem specified by values of σ which do not belong to the mesh Σ must be determined by solving an equation of the type (14), and those must be selected which satisfy the constraint (20).

The problem under investigation can finally be solved by the method of regularization [16] (hence, knowledge of the quantities δ, C_{min}, and C_{max} is not obligatory), where in place of the traditional mesh functions $C_0^*(\xi)$ functions of the spaces $\Psi^{(2)}$ and $\Psi^{(3)}$ are used. Approximating the integral operator is not performed and the functional to be minimized –

$$\sum_{j=1}^{n} [\tilde{C}(x_j) - C^*(x_j)]^2 + \bar{\alpha} \int_{\alpha}^{\beta} (C_0^*(\xi))'' \, d\xi$$

– for fixed σ is a quadratic functional in the variables A_i.

The solution of the problem reduces to absolute minimization of this functional in a mesh of values of the regularization parameter $\bar{\alpha}$, and the selection of the best of these values can be realized by the principle of the quasioptimal parameter [17] without requiring knowledge of δ:

$$\bar{\alpha}_{k.o} = \min_{\bar{\alpha} \in \Omega} \{\Delta = \| C_0^*(\xi;\, \bar{\alpha}_{j+1}) - C_0^*(\xi;\, \bar{\alpha}_j) \|\},$$
$$\Omega = \{\bar{\alpha}_j\}_0^{\infty}, \quad \bar{\alpha}_{j+1} = \varkappa \bar{\alpha}_j; \ \bar{\alpha}_0, \ \varkappa > 0, \tag{22}$$

where the domain of definition of the function in (22) is the segment $[\alpha, \beta]$. The presence of the constraint (20) admits of a more purposeful selection of $\bar{\alpha}$ and the information (21) of the natural regularization parameter L. Let us note that the regularization algorithm in the problem (3) is used in [18].

NOTATION

C is the concentration;
D is the coefficient of diffusion;
C_0 is the initial distribution of concentration;
x is a coordinate;
ξ is a coordinate;
τ is the time.

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