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Problems of heat, mass and charge transfer with discontinuous solutions

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Typical problems with solutions characterised by first-kind discontinuities occurring at interfaces of layered inhomogeneous media are considered with respect to second-order differential equations in partial derivatives. Direct, inverse and mixed types of solution discontinuities are considered. Presented are generalised formulations of problems under consideration, having discontinuous solutions and allowing a uniform description of the processes of heat, mass and charge transfer in multilayer media. Homogeneous difference schemes built on the basis of generalised solutions, which are illustrated by test problems with analytical solutions, are given.

Key words: heat, mass and charge transfer; discontinuous solutions; finite-difference schemes; generalized solutions

1 Introduction

Discontinuities of distributed characteristics of fields (temperature, concentration, electric potential, pressure, etc.) in mathematical descriptions of different physical processes can be caused by different factors. The most common version of a discontinuous solution applies to the development of mathematical models of the transfer processes in layered inhomogeneous media, having a thin (compared with characteristic geometrical sizes of the media), low-permeable interlayer at contact boundary between the media. When contact problems of this kind are solved numerically, including thin interlayers into the region of solutions, it requires an unjustifiable mesh refinement. Therefore, a simplified model of an interlayer is developed for such cases, as this model allows this interlayer to be excluded from the region of solution of a differential problem. Conditions of conjunction of a solution at interface between the layered inhomogeneous media, present in a classic statement of the problems of heat, mass and charge transfer, require approximation of normal components of vectors of the specific substance flows in the case of the numerical

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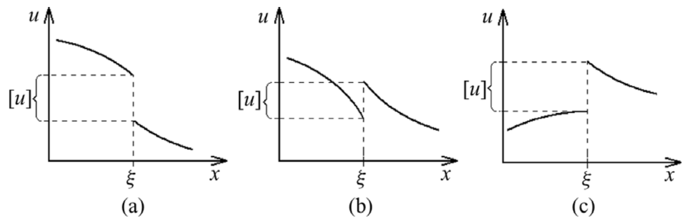

FIGURE 1. Schemes of discontinuity of solution at point (a) direct jump, (b) inverse jump and (c) combined jump.

solution, which involves certain difficulties in construction and realisation of calculation algorithms. From this standpoint, it is expedient to reformulate the classic statements of the corresponding problems, so that the transfer processes can be uniformly described for the entire multilayer system as a whole, and that the interface conditions as an attribute of mathematical formulation of a problem can be excluded. This study is dedicated to the development of these generalised models for characteristic problems of heat, mass and charge transfer with a discontinuous solution.

2 Discontinuous solution models

The development of models of an interlayer is based, as a rule, on a quasi-unidimensional character of the process of transfer of a substance through the interlayer. A characteristic example of a model of the interlayer is a problem of a non-ideal heat contact of two heat-conducting bodies [1] . The model of the interlayer of non-ideally contacting media is developed on the basis of an assumption that heat transfer through this interlayer occurs in a normal direction to the contact boundary, and that it is unidimensional and stationary. With these hypotheses, a jump of temperature $[T]_\Gamma$ (hereinafter the jump of function $f(\bar{x})$ at boundary Γ is designated as $[f]_\Gamma$) at interfaces between the interlayer and the heat-conducting media it separates is proportional to projection of the heat flow vector, $\vec{w} = -\lambda\vec{\nabla}T$, onto a direction of normal $\vec{n}$ to boundary Γ, i.e.

$$[T]_\Gamma = -Rw_n|_\Gamma, \tag{2.1}$$

where $R = \delta_p/\lambda_p$ stands for the surface heat resistance determined through thickness δ_p and thermal conductivity λ_p of the interlayer. In condition (2.1), $[T]_\Gamma$ means $[T]_\Gamma = T|_{\Gamma_+} - T|_{\Gamma_-}$, where Γ_+ is the side of surface Γ looking in the direction of normal $\vec{n}$. The validity of using of such type of effective boundary conditions was studied recently in [2], where the generalised boundary condition of a kind of non-ideal thermal contact was derived from the asymptotic theory.

Note that expression (2.1) is invariant for selection of the direction of normal $\vec{n}$. Specific peculiarity of the model of a non-ideal contact of type consists in the fact that $\operatorname{sign}[T]_\Gamma = \operatorname{sign}(\vec{\nabla}T)_n|_\Gamma$. Therefore, $R > 0$ in condition (2.1). We will call this type of solution as discontinuity a direct jump (Figure 1(a)), in contrast to the inverse jump, which will be considered below. In practical applications, the interlayer may have a complex internal structure with heat-conducting properties, which are hard to identify. In such cases, the heat resistance of the interlayer R is determined experimentally. Contact

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problems of thermal conductivity with such type of the interlayer model are not an exception. Similar problems arise in subsurface hydrodynamics, which studies filtration of subterranean waters through thin, low-permeability interlayers, in contact problems of interaction of the electric fields in layered heterogeneous media and in other applications.

The other variant of discontinuity of the unknown function at an internal boundary of the solution region is a case of the problem associated with calculation of scalar potential φ of the electromagnetic field in the 'anode–arc plasma' system. A thin near-anode layer exists at the interface between the metal anode and electric arc plasma. According to the generalised Ohm's law, the electric current in this layer can be directed opposite to the vector of intensity of the electric field [3]. A simplified model of the near-anode layer is suggested in [4]. According to this model, jump $[\varphi]_\Gamma$ of potential of the electric field in this layer is in a non-linear dependence upon the value of component $j_n|_\Gamma$, normal to the anode boundary, of the vector of electric current density, $\vec{j} = -\sigma\vec{\nabla}\varphi$, where σ is the specific electrical conductivity, i.e.

$$[\varphi]_\Gamma = G(j_n|_\Gamma). \tag{2.2}$$

It is assumed in this case that $j_n|_\Gamma$ remains continuous at boundary Γ of contact of the anode with plasma. Unlike model (2.1) of a non-ideal contact, model of the anode layer (2.2) does not only make the problem of calculation of potential φ non-linear but also leads to the other type of the solution jump, i.e. the so-called inverse jump, the unidimensional variant of which is schematically shown in Figure 1(b). In this case, the following relationship is met between the signs of $[\varphi]_\Gamma$ and $(\vec{\nabla}\varphi)_n|_\Gamma$: sign $[\varphi]_\Gamma = -\text{sign}(\vec{\nabla}\varphi)_n|_\Gamma$, and it is this relationship that justifies the 'inverse jump' term.

The problem of distributive diffusion gives another example of the solution jump. This problem arises in the description of segregation of solute impurities in the processes of solidification of alloys. Within the frames of the so-called modified Stephan's problem [5], the condition of conjunction of solutions at interface Γ between the phases has the following form:

$$C_S|_{\Gamma_-} = \chi C_L|_{\Gamma_+}, \tag{2.3}$$

where C_S and C_L are the concentrations of an impurity in the solid and liquid phases, respectively, and χ is the distribution coefficient (segregation coefficient), which meets condition $0 < \chi < 1$ for the majority of alloys. If the lines on a phase diagram of a binary alloy are straight, then $\chi = const$, otherwise $\chi = \chi(C)$ and the problem becomes non-liner. In what follows, we will consider $\chi = const$, which corresponds to a linearised phase diagram. Condition (2.3) can be re-written to have the following form: $[C]_\Gamma = (1-\chi)C_L|_{\Gamma_+}$, i.e. at interface Γ, the jump of the concentrations is proportional to the concentration of the impurity in one of the phases. We will call this jump as a combined jump, meaning that it is direct with respect to the direction of the concentration gradient in the solid phase, and inverse with respect to the gradient in the liquid phases (see Figure 1(c)).

3 Generalised formulations of problems with discontinuous solutions

Let R_n be the n-dimensional Euclidean space, $\bar{x} = \{x_1, x_2, \ldots, x_n\}$ – the Cartesian coordinates, $\Omega \subset R_n$ – the region of solution of a problem, which is assumed to be two-layer to simplify the writing: $\Omega = \Omega_1 \cup \Omega_2$, and Γ – interface between sub-regions Ω_1 and Ω_2. Identify variables relating to sub-regions Ω_1 and Ω_2 by indices 1 and 2, respectively. Designate the unknown solution of the problem as $u(\bar{x})$, and the specific flow of a substance as $\vec{q}(\bar{x})$. Consider function $u(\bar{x})$ to be sufficiently smooth everywhere in Ω, except maybe for interface Γ, where it experiences jump $[u(\bar{x})]_\Gamma$. The jump $[u(\bar{x})]_\Gamma$ is assumed to be a continuous function of coordinates of interface Γ. Define the specific flow in each of the sub-regions Ω_1 and Ω_2 as follows: $\vec{q}_m = -k_m \vec{\nabla} u_m, m = 1, 2$, assuming that operator $\vec{\nabla}$ is determined in classic interpretation as a function of point $\bar{x} \in \Omega_1, \Omega_2$. Assume also that coefficients $k_m(\bar{x}), m = 1, 2$ are sufficiently smooth such that they meet the condition $k_m(\bar{x}) \geqslant C > 0$. Assume that functions $u_m(\bar{x})$ (e.g. temperature, potential of the electric field) in each of the sub-regions Ω_m meet the following equations:

$$\nabla(k_m \vec{\nabla} u_m) = f_m(\bar{x}), \ \bar{x} \in \Omega_m, \ m = 1, 2. \tag{3.1}$$

Assume that the specific flow vector component normal to Γ is continuous, i.e.

$$q_{1n}|_{\Gamma_+} = q_{2n}|_{\Gamma_-}. \tag{3.2}$$

For the non-ideal contact model (2.1), the second condition of conjunction of solutions at interface Γ can be written in the following form:

$$[u]_\Gamma = -R(\vec{x}) q_n|_\Gamma, \ \vec{x} \in \Gamma. \tag{3.3a}$$

In a linear statement of the problem for calculation of potential of the electric field, in contrast to (2.2), assume that the difference of potentials $[u]_\Gamma$ is set at interface Γ as a function of coordinates of interface Γ:

$$[u]_\Gamma = g(\vec{x}), \ \vec{x} \in \Gamma. \tag{3.3b}$$

Assume that certain boundary conditions, the specific form of which is of no importance for further description, are met at external boundary $\partial\Omega$ of region Ω, and suppose that there is also a unique solution of the problem in the classic statement. Define functions $u(\bar{x})$, $\vec{q}(\bar{x})$, $\frac{\partial u}{\partial x_i}$, $k(\bar{x})$ in Ω, which exist everywhere in Ω as functions of a point, except for interface Γ, in the following form: $\psi(\bar{x}) = \psi_m(\bar{x})$, $\bar{x} \in \Omega_m$, where $\psi(\bar{x})$ is one of the above functions. The generalised partial derivatives $\frac{D}{Dx_i}$ of function $u(\bar{x})$ in region Ω are defined as follows:

$$\frac{Du}{Dx_i} = \frac{\partial u}{\partial x_i} + [u]_\Gamma^{(i)} \gamma_i \delta(\Gamma), \ \bar{x} \in \Gamma, \tag{3.4}$$

where $[u]_\Gamma^{(i)}$ is the solution jump reached by function $u(\bar{x})$ in a direction of axis $0x_i$ (assume further on that $[u]_\Gamma^{(i)} = [u]_\Gamma$, $i = \overline{1, n}$), $\gamma_i = \cos(\vec{n}, \vec{x}_i)$ are the direction cosines of normal to Γ, $\delta(\Gamma)$ is the Dirac's delta-function concentrated on hypersurface Γ of the $(n-1)$th measure. Using (3.4), introduce a generalised gradient $GRAD_-$ of discontinuous function $u(\bar{x})$ in Ω:

$$GRAD_- u = \vec{\nabla} u + \vec{n} \, [u]_\Gamma \, \delta(\Gamma). \tag{3.5}$$

As $-k\vec{\nabla}u = \vec{q}(\bar{x})$, it follows from (3.5) that

$$GRAD\_u = -\rho\vec{q} + \vec{n}\,[u]_\Gamma\,\delta(\Gamma), \tag{3.6}$$

where $\rho(\bar{x}) = k^{-1}(\bar{x})$ is the specific resistance of a medium.

3.1 Non-ideal heat contact (direct jump)

Eliminate $[u]_\Gamma$ from (3.6) using the contact model (3.3a). Thus, we will have: $-GRAD\_u = \rho\vec{q} + \vec{n}Rq_n\delta(\Gamma)$. Vector $\vec{n}q_n$ can be described as follows: $\vec{n}q_n = P\vec{q}$, where P is the second-rank tensor, components $p_{i,j}$ of which can be expressed in terms of the direction cosines of normal $\vec{n}$ as follows: $p_{i,j} = \gamma_i\gamma_j$. Finally, it holds that

$$-GRAD\_u = \Xi\vec{q}, \tag{3.7}$$

where $\Xi = E\rho + R\delta(\Gamma)P$, and E is the unit tensor. Relationship (3.7) can be interpreted as a generalised phenomenological law (Fourier's, Fick's, Darcy's or Ohm's law) formulated for discontinuous potential $u(\bar{x})$. As follows from (3.7), the non-ideal contact of conducting media induces local anisotropy of conducting properties of a medium at contact boundary Γ (orthotropy, if Γ is a plane parallel to coordinate axes, or if the direction of normal to Γ coincides with the direction of the specific flow vector). Note that the phenomenological law in a classic statement permits two equivalent forms of writing down of the specific flow: in terms of specific conductivity ($\vec{q} = -k\vec{\nabla}u$), or in terms of specific resistance ($\rho\vec{q} = -\vec{\nabla}u$) of a medium. Using the first of them in the conservation law, $-\nabla \cdot \vec{q} = f$, yields as a rule the second-order equation of the type (3.1). The generalised phenomenological law (3.7) permits only one form, as the function inverse to the delta function has no mathematical meaning [6]. In this connection, the generalised statement of the problem for the calculation of the discontinuous potential should be based on a mathematical description of the transfer process, which is absolutely natural from the physical standpoint, in the form of a system of the first-order equations, one of which (scalar) is a generalised law of conservation of a substance, and the second (vector) is a generalised phenomenological law:

$$\begin{cases} -DIV_+\vec{q} = f, \\ -GRAD\_u = \Xi\vec{q}, \end{cases} \tag{3.8}$$

where DIV_+ is the divergence operator determined for the class of vector-functions $\vec{q}(\bar{x}) \in \vec{W}_2^1(\Omega)$. Use of a generalised divergence operator in (3.8) is required because components $q_i(\bar{x})$ of vector $\vec{q}(\bar{x})$ at interface Γ are the discontinuous functions. Therefore, the generalised solution of the problem of a non-ideal contact implies a pair of functions, i.e. vector $\vec{q}(\bar{x})$ and scalar $u(\bar{x})$, which meet equation (3.8) and corresponding boundary conditions in terms of the theory of generalised functions (we deliberately omit here the required mathematical formalism, trying to maintain a physical clarity of the formulations suggested). The generalised formulation of the non-stationary problem of a non-ideal heat contact of two media can naturally result from (3.8), provided that the non-stationary term $c_p \frac{\partial u}{\partial t}$, where c_p is the specific heat and t is the time, is taken into account in the law of conservation of energy.

Equation (3.8) also has a useful result for consideration of the problem with boundary conditions of the third kind. Let a heat exchange (heat transfer) condition be set at boundary $\partial\Omega$ following the Newton–Richman law:

$$-\lambda \frac{\partial u}{\partial n}|_{\partial\Omega} = \alpha(u|_{\partial\Omega} - u_C), \tag{3.9}$$

where u_C is the temperature of an external medium, where the heat exchange process takes place. Condition (3.9) can be interpreted as a non-ideal heat contact of a body with the external medium, and contact heat resistance $R = \alpha^{-1}$ can be allowed for in the generalised Fourier's law (3.7) by replacing here the boundary condition of the third kind (3.9) by the boundary condition of the first kind, $u|_{\partial\Omega} = u_C$.

3.2 Charge transfer in 'anode–arc plasma' system (inverse jump)

In the case of an inverse solution jump, which, for example, forms an anode layer at the arc plasma and metal anode interface, the generalised equations in a linear statement, which describe distribution of potential of the electric field in such a two-layer medium, can be written down, using expression (3.6) as a generalised Ohm's law, as follows:

$$\begin{cases} -DIV_{+}\vec{q} = f, \\ -GRAD_{-}u = \rho\vec{q} - \vec{n}[u]_{\Gamma}\,\delta(\Gamma). \end{cases} \tag{3.10}$$

It is implied in (3.10) that the potential jump $[u]_\Gamma$ at the boundary Γ is set as a function of the boundary coordinates of Γ, in accordance with (3.3b).

The generalised solution of the system of equations (3.10), in analogy with (3.8), implies the vector of current density, $\vec{q}(\bar{x})$, and scalar potential of the electromagnetic field, $u(\bar{x})$, which meet equations (3.10) in terms of the theory of generalised functions, as well as boundary conditions set at $\partial\Omega$. It is assumed in (3.10) that $[u]_\Gamma$, being a function of coordinates of interface Γ, is continuous at Γ. When solving real problems of charge transfer in the 'anode–arc plasma' system, it is necessary to allow for non-linear dependence (2.2) of the jump of potential on the current density. The iterative process because of the non-linearity implies solving of linear equations of the type (3.10) at each iteration.

3.3 Segregation of impurity at interface between phases (inverse and combined jump)

A characteristic example of the problem with a jump, the type of which depends upon the time, is a non-stationary problem of segregation of an impurity during solidification. Consider the generalised formulation of such a problem, first in the one-dimensional statement. Let $C_S(x,t)$ and $C_L(x,t)$ be the concentrations of a solute impurity in the solid and liquid phases, respectively, and $x = \xi(t)$ is interface between the phases, the law of motion of which is assumed to be known. Assume that transfer of substance in each of the co-existing phases occurs by the diffusion mechanism

$$\frac{\partial C_S}{\partial t} = D_S \frac{\partial^2 C_S}{\partial x^2}, \quad 0 < x < \xi(t); \quad \frac{\partial C_L}{\partial t} = D_L \frac{\partial^2 C_L}{\partial x^2}, \quad \xi(t) < x < l, \tag{3.11}$$

where D_S and D_L are the diffusion coefficients. The following interface conditions for the concentration fields in the solid and liquid phases are met at the interface between the phases, $x = \xi(t)$:

$$\begin{cases} C_S(\xi - 0, t) = \chi C_L(\xi + 0, t), \\ D_S \left.\dfrac{\partial C_S}{\partial x}\right|_{x=\xi(t)-0} - D_L \left.\dfrac{\partial C_L}{\partial x}\right|_{x=\xi(t)+0} = \dfrac{d\xi}{dt}\left[C_L(\xi + 0, t) - C_S(\xi - 0, t)\right], \end{cases} \tag{3.12}$$

where $\chi = const$ is the distribution coefficient. The first of them corresponds to condition (2.3), and the second corresponds to a local law of conservation of mass at the interface between the phases. In contrast to the cases considered above, not only the unknown function, but also the specific mass flow is discontinuous in the problem of segregation of an impurity at the interface between the media, discontinuity of the flow being proportional to discontinuity of the solution. The discontinuity of the solution in the case under consideration is removable. For this, add new unknown function $u(x,t)$, i.e. potential of mass transfer

$$u(x,t) = \begin{cases} u_S(x,t), \; 0 < x < \xi(t), \\ u_L(x,t), \; \xi(t) < x < l, \end{cases}$$

and re-write equations (3.11) and (3.12) allowing for function $u(x,t)$

$$\frac{\partial u_S}{\partial t} = \frac{\partial}{\partial x}\left(D_S \frac{\partial u_S}{\partial x}\right), \quad 0 < x < \xi(t); \quad \frac{1}{\chi}\frac{\partial u_L}{\partial t} = \frac{\partial}{\partial x}\left(\frac{D_L}{\chi}\frac{\partial u_L}{\partial x}\right), \quad \xi(t) < x < l, \tag{3.13}$$

$$u_S(\xi - 0, t) = u_L(\xi + 0, t); \quad D_S \left.\frac{\partial u_S}{\partial x}\right|_{x=\xi(t)-0} - \frac{D_L}{\chi}\left.\frac{\partial u_L}{\partial x}\right|_{x=\xi(t)+0} = \frac{d\xi}{dt}\frac{1-\chi}{\chi}u(\xi, t). \tag{3.14}$$

Set functions $\zeta(x,t)$ and $D_{SL}(x,t)$ in interval $(0,l)$ as follows:

$$\zeta(x,t) = \begin{cases} 1, 0 < x < \xi(t) \\ \dfrac{1}{\chi}, \xi(t) < x < l \end{cases}; \quad D_{SL}(x,t) = \begin{cases} D_S, \; 0 < x < \xi(t) \\ \dfrac{D_L}{\chi}, \; \xi(t) < x < l \end{cases}.$$

Function $\zeta(x,t)$ can be interpreted as a relative solubility of the co-existing phases. Introduce the generalised partial derivatives $\frac{D}{Dx}$, $\frac{D}{Dt}$ of the function that experiences discontinuities of the first kind by spatial variable x and time t. The discontinuity of the flows of the mass transfer potential in condition (3.14) can be interpreted as a mass source concentrated at boundary $x = \xi(t)$. Therefore, the generalised equation of mass transfer in the entire two-phase system can be written down in the following form:

$$\zeta \frac{\partial u}{\partial t} = \frac{D}{Dx}\left(D_{SL}\frac{\partial u}{\partial x}\right) - \frac{d\xi}{dt}\frac{1-\chi}{\chi}u(\xi, t)\delta(x - \xi(t)), \quad 0 < x < l. \tag{3.15}$$

Here $\delta(x - \xi(t))$ is the δ-function concentrated at point $x = \xi(t)$.

Express $\zeta(x,t)$ as $\zeta(x,t) = 1 + \frac{1-\chi}{\chi}\theta(x-\xi(t))$, where $\theta(x-\xi(t))$ is the unit Heaviside function. As $\frac{D\theta}{Dt} = \frac{d\xi}{dt}\delta(x-\xi(t))$, $\frac{D\zeta}{Dt} = \frac{d\xi}{dt}\frac{1-\chi}{\chi}\delta(x-\chi(t))$. Hence, allowing for the fact that $u(\xi,t)\delta(x-\xi(t)) = u(x,t)\delta(x-\xi(t))$, the generalised equation of mass transfer can be written down in the interval $(0,l)$ in a unified form by excluding the interface conditions (3.14) as an element of the mathematical statement of the problem

$$\frac{D}{Dt}(\zeta u) = \frac{D}{Dx}\left(D_{SL}\frac{\partial u}{\partial x}\right), \quad 0 < x < l. \tag{3.16}$$

In a general case of distribution diffusion in the M-phase system, the equation of mass transfer will be maintained in form (3.16) if the relative solubility is determined in a form of $\zeta_m = \left[\prod_{i=0}^{m}\chi_i\right]^{-1}$, $m = \overline{0,M}$, $\chi_0 = 1$, and if the unknown function is replaced by $u_m = \chi_m C_m$, $\xi_{m-1} < x < \xi_m$. For the multi-dimensional modified Stephan problem, set configuration of the solidification front and its movement speed. In this case, the form of writing down of the equation of mass transfer remains identical to (3.16)

$$\frac{D}{Dt}(\zeta u) = DIV_{-}\left(D_{SL}GRAD_{+}u\right).$$

Here DIV_{-} is the extension in continuity of the ∇ operator to a class of piecewise continuous (piecewise differentiable) vector functions, and $GRAD_{+}$ is the gradient operator determined in a class of functions $u(\bar{x}) \in W_2^1(\Omega)$.

4 Homogeneous difference schemes based on generalised equations

In this section, we will limit ourselves to the development of difference schemes for sufficiently simple one-dimensional test problems. However, the main approaches to the development of methods for finding numerical solutions will also be extended to a case of the more complex multi-dimensional problems. In order to estimate the actual accuracy of such schemes, consider three characteristic test problems having an exact solution.

4.1 Non-ideal contact

Formulate the one-dimensional stationary problem of a non-ideal contact as a first model example. Consider the following problem for interval $[0,1]$ according to the generalised statement (3.8)

$$-\frac{dq}{dx} = f(x), \quad -\frac{Du}{Dx} = \tilde{\rho}(x)q(x), \quad 0 < x < 1; \qquad u(0) = u(1) = 0. \tag{4.1}$$

Here $\tilde{\rho}(x) = \rho(x) + R\delta(x-\xi)$, where $\rho(x) \in L_\infty(0,1)$, $\rho(x) \geqslant C > 0$; $\xi \in (0,1)$ is the coordinate of the boundary of a non-ideal contact, and $R > 0$ is the contact resistance. Use mesh $\omega_h = \{x_i = ih,\ i = \overline{0,N},\ Nh = 1\}$ in region $[0,1]$. Integrating the first of equations (4.1) in region $[x_i - 0.5h,\ x_i + 0.5h]$ yields a mesh analog of the conservation law in the following form:

$$-\frac{q(x_i+0.5h) - q(x_i-0.5h)}{h} = \frac{1}{h}\int_{x_i-0.5h}^{x_i+0.5h} f(x)dx. \tag{4.2}$$

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Approximate equalities follow from the second equation of (4.1)

$$q(x_i + 0.5h) \approx -a_{i+\frac{1}{2}} \frac{u(x_{i+1}) - u(x_i)}{h}, \quad q(x_i - 0.5h) \approx -a_{i-\frac{1}{2}} \frac{u(x_i) - u(x_{i-1})}{h}, \tag{4.3}$$

where $a_{i+\frac{1}{2}} = \left[\frac{1}{h}\int_{x_i}^{x_{i+1}} \rho(x)dx + \frac{R}{h}\beta_i\right]^{-1}$, $\beta_i = 1, \xi \in (x_i, x_{i+1})$, $\beta_i = 0, \xi \notin (x_i, x_{i+1})$. Derive the following difference scheme from (4.2) and (4.3) and from the boundary conditions:

$$\frac{1}{h}\left[a_{i+\frac{1}{2}} \frac{y_{i+1} - y_i}{h} - a_{i-\frac{1}{2}} \frac{y_i - y_{i-1}}{h}\right] = \varphi_i, \quad i = \overline{1, N-1}; \quad y_0 = 0, \ y_N = 0, \tag{4.4}$$

where the solution of the difference problem is expressed in terms of y_i, and $\varphi_i = \frac{1}{h}\int_{x_i - 0.5h}^{x_i + 0.5h} f(x)dx$. The resulting difference scheme is absolutely identical in the form of writing down to the difference scheme for a smooth solution, the non-ideal contact being allowed for in coefficients $a_{i+\frac{1}{2}}$ of the mesh equation, which can be readily imparted a physical meaning if we take into account that the integral in square brackets is the resistance of a mesh cell, which corresponds to a series connection of conductors. Let $u_i^{(h)} = \frac{1}{h}\int_{x_i}^{x_{i+1}} u(x)dx$ be the projection of a solution of the differential problem onto the mesh, and $z_i = y_i - u_i^{(h)}$ – the error of the numerical solution. It can be shown that inequality $\|z\|_C \leqslant Mh$, where $M = const$, takes place in the above class of coefficients. Therefore, difference scheme (4.4) is uniformly reduced to the generalised solution of problem (4.1) and has the first order of accuracy. In order to prove this inequality, the approximation error is estimated in a weak summatory metric [7], the involvement of which is related to the fact that the local approximation error in the vicinity of discontinuity of the solution is $O\left(\frac{1}{h}\right)$. Allowing for the fact that the number of the mesh points with an abnormal approximation error remains finite at $h \to 0$, it results in the above estimate of accuracy of the difference scheme. Note that difference scheme (4.4) is accurate at $f(x) \equiv 0$. In a general case, where $\tilde{\rho}(x) \in W_2^{-1}(0,1)$, $f(x) \in L_2(0,1)$, $u(x) \in L_2(0,1)$, $q(x) \in W_2^1(0,1)$, it is possible to prove only the convergence of the difference scheme (without establishing the order of accuracy).

Now formulate the one-dimensional non-stationary problem of thermal conductivity with a discontinuous solution by the type of a non-ideal heat contact as follows:

$$c_1 \frac{\partial u_1}{\partial t} = k_1 \frac{\partial^2 u_1}{\partial x^2}, \quad u_1(x,0) = 1, \quad x > 0;$$

$$c_2 \frac{\partial u_2}{\partial t} = k_2 \frac{\partial^2 u_2}{\partial x^2}, \quad u_2(x,0) = 0, \quad x < 0;$$

$$k_1 \frac{\partial u_1}{\partial x}\bigg|_{x=0} = k_2 \frac{\partial u_2}{\partial x}\bigg|_{x=0}; \quad k_1 \frac{\partial u_1}{\partial x}\bigg|_{x=0} = \alpha[u]_{x=0}; \quad \lim_{x\to\infty} u_1(x,t) = 1; \quad \lim_{x\to-\infty} u_2(x,t) = 0,$$

assuming that k_1, k_2, c_1, c_2 and α are constants. The problem formulated has an exact solution [1]. Write down, in analogy with (4.4), an implicit difference equation for the non-stationary problem of thermal conductivity with a non-ideal contact

$$c_i \frac{y_i^{(j+1)} - y_i^{(j)}}{\tau} = \frac{1}{h}\left[a_{i+\frac{1}{2}} \frac{y_{i+1}^{(j+1)} - y_i^{(j+1)}}{h} - a_{i-\frac{1}{2}} \frac{y_i^{(j+1)} - y_{i-1}^{(j+1)}}{h}\right], \tag{4.5}$$

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Table 1. *Exact (u) and numerical (y) solution of problem of non-ideal contact*

	$t = 10$ s		$t = 20$ s		$t = 100$ s	
x	u	y	u	y	u	y
−1	0.1070	0.1038	0.1825	0.1797	0.3374	0.3369
−7/8	0.1279	0.1240	0.2035	0.2005	0.3503	0.3498
−3/4	0.1515	0.1469	0.2258	0.2228	0.3634	0.3629
−5/8	0.1778	0.1727	0.2494	0.2464	0.3766	0.3762
−1/2	0.2066	0.2013	0.2742	0.2713	0.3900	0.3896
−3/8	0.2381	0.2327	0.3002	0.2975	0.4035	0.4031
−1/4	0.2719	0.2668	0.3272	0.3248	0.4171	0.4168
−1/8	0.3079	0.3032	0.3551	0.3530	0.4308	0.4305
0	0.6544	0.6505	0.6162	0.6148	0.5554	0.5552
1/8	0.6922	0.6876	0.6449	0.6433	0.5692	0.5689
1/4	0.7281	0.7230	0.6728	0.6710	0.5829	0.5826
3/8	0.7619	0.7563	0.6998	0.6978	0.5965	0.5962
1/2	0.7934	0.7873	0.7258	0.7236	0.6100	0.6097
5/8	0.8222	0.8159	0.7506	0.7482	0.6234	0.6231
3/4	0.8485	0.8419	0.7742	0.7716	0.6366	0.6363
7/8	0.8721	0.8653	0.7965	0.7937	0.6497	0.6493
1	0.8930	0.8861	0.8175	0.8145	0.6626	0.6622

where τ is the time step. Assume for numeric calculations that $c_1 = c_2 = 1.0$; $k_1 = k_2 = 0.1$; $h = \frac{1}{8}$; $\tau = 1.0$, and place the non-ideal contact boundary $x = 0$ at a mesh point. Boundary conditions for equation (4.5) were set at a sufficiently large distance on both sides of the non-ideal contact boundary. As follows from Table 1, which gives the exact and calculated values of the unknown functions for different time moments, on quite coarse time and space meshes, the numerical solution coincides with the solution of a differential problem with a good accuracy.

4.2 Segregation of impurity

Consider the problem of segregation of an impurity in the following model statement:

$$\begin{gathered}
\frac{\partial C_1}{\partial t} = D_1 \frac{\partial^2 C_1}{\partial x^2}, \quad -\infty < x < \xi(t); \\
\frac{\partial C_2}{\partial t} = D_2 \frac{\partial^2 C_2}{\partial x^2}, \quad x > \xi(t), \quad \xi(t) = vt; \\
D_1 \frac{\partial C_1}{\partial x}\bigg|_{x=\xi(t)-0} - D_2 \frac{\partial C_2}{\partial x}\bigg|_{x=\xi(t)+0} = v[C]_{x=\xi}; \quad C_1(\xi - 0, t) = \chi C_2(\xi + 0, t); \qquad (4.6) \\
\lim_{x\to-\infty} C_1(x,t) = C_1^0; \quad \lim_{x\to\infty} C_2(x,t) = C_2^0; \\
C_1(x,0) = C_1^0 \quad x < \xi(0); \quad C_2(x,0) = C_2^0, \quad x > \xi(0).
\end{gathered}$$

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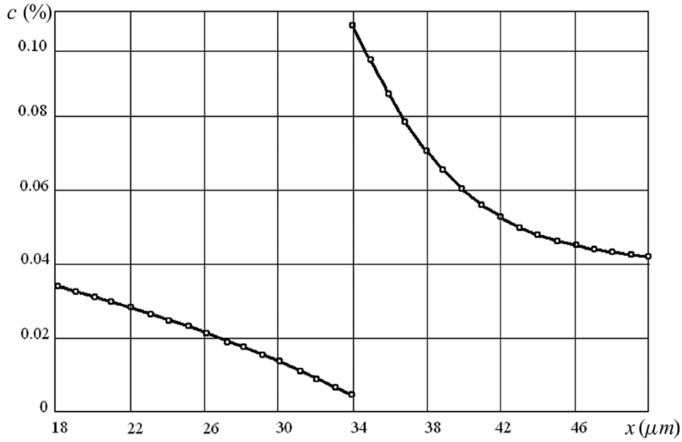

FIGURE 2. Distribution of sulphur in solidification of iron–carbon steel at the initial stage of solidification (solid line shows exact solution, and open circles ∘ show the numerical solution).

This problem also has an analytical solution [8]. Write down an implicit difference equation for the generalised equation of mass transfer (3.16)

$$\frac{\zeta_i^{(j+1)} y_i^{(j+1)} - \zeta_i^{(j)} y_i^{(j)}}{\tau} = \frac{1}{h}\left[a_{i+\frac{1}{2}} \frac{y_{i+1}^{(j+1)} - y_i^{(j+1)}}{h} - a_{i-\frac{1}{2}} \frac{y_i^{(j+1)} - y_{i-1}^{(j+1)}}{h}\right], \tag{4.7}$$

where $\zeta_i^{(j+1)} = \frac{1}{h}\int_{x_i-0.5h}^{x_i+0.5h} \zeta(x, t_{j+1})dx$, $a_{i+\frac{1}{2}} = \left[\frac{1}{h}\int_{x_i}^{x_{i+1}} \frac{dx}{D_{SL}(x,t_{j+1})}\right]^{-1}$. With the numerical solution, the mesh problem was solved for a region of a limited length, which was selected so that the effect of limitation of the region was negligible. Numerical parameters of the model were set for conditions of segregation of sulphur during solidification of an iron–carbon steel: $D_1 = 10^{-11}\,\mathrm{m^2\,s^{-1}}$, $D_2 = 10^{-9}\,\mathrm{m^2\,s^{-1}}$, $\chi = 0.05$, $C_1^0 = C_2^0 = 0.04$ %, $v = 10^{-4}\,\mathrm{m\,s^{-1}}$; and the selected numerical parameters were as follows: $h = 10^{-7}\,\mathrm{m}$, $\tau = 10^{-3}\,\mathrm{s}$. Figure 2 shows comparison of the exact and numerical solutions of problem (4.6) at the initial stage of the solidification process ($t = 0.04\,\mathrm{s}$), when the jump of the solution is inverse. With the numerical solution of the problem, it was assumed that boundary $x = \xi(t)$ was at a mesh point and moved by one time step exactly to one point on the spatial coordinate. As seen from the calculation results, difference scheme (4.7) provides a sufficiently high accuracy of the numerical solution.

Figure 3 shows numerical solution of problem (4.6) at the final stage of solidification, where a combined solution jump is formed.

4.3 Current transfer in 'anode–arc plasma' system

Consider a one-dimensional variant of generalised formulation (3.10) of the problem of distribution of potential and electric field in the 'anode–arc plasma' system

$$-\frac{dq}{dx} = 0; \quad \frac{Du}{Dx} = -\rho q + [u]_\xi \delta(x - \xi), \quad 0 < x < l; \quad u(0) = 0, \quad u(l) = u_0, \tag{4.8}$$

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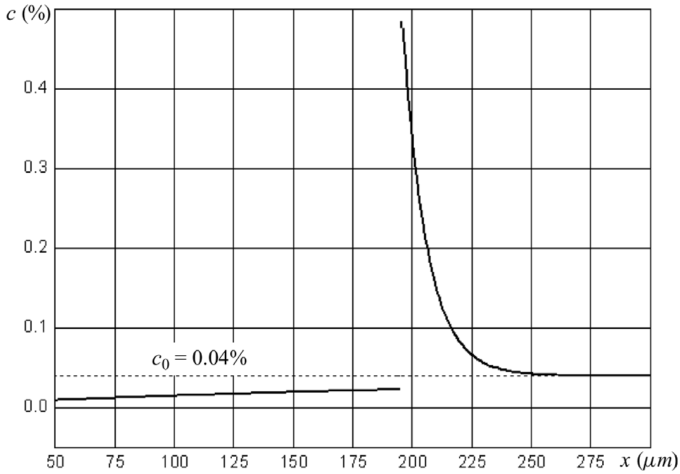

FIGURE 3. Distribution of sulphur in solidification of iron–carbon steel at the final stage of solidification.

where q is the current density, u is the potential of the electric field, $\rho = \rho(x)$ is the specific electrical resistance of medium, $\xi \in (0, l)$ is the position of the metal-plasma interface and $[u]_\xi$ is the potential jump at this interface (anode barrier). In a case where $\rho(x) = \rho_1 = const$, $0 < x < \xi$ and $\rho(x) = \rho_2 = const$, $\xi < x < l$, problem (4.8) has a simple analytical solution:

$$u(x) = \begin{cases} -q\rho_1 x, & 0 < x < \xi, \\ -q(\rho_1\xi + \rho_2(x - \xi)) + [u]_\xi, & \xi < x < l, \end{cases} \tag{4.9}$$

where $q = \frac{[u]_\xi - u_0}{\rho_1\xi + \rho_2(l - \xi)}$. It is just enough to modify a bit the computations of (4.2) and (4.3) to obtain a difference analog of problem (4.8) on the mesh ω_h:

$$\frac{1}{h}\left[a_{i+\frac{1}{2}}\frac{y_{i+1} - y_i}{h} - a_{i-\frac{1}{2}}\frac{y_i - y_{i-1}}{h}\right] = \varphi_i, \quad i = \overline{1, N-1}; \quad y_0 = 0, \quad y_N = u_0, \tag{4.10}$$

where $a_{i+\frac{1}{2}} = \left[\frac{1}{h}\int_{x_i}^{x_{i+1}} \rho(x)dx\right]^{-1}$. Let $x_m < \xi < x_{m+1}$, then the right part of mesh equation (4.10) can be calculated as follows: $\varphi_i = 0$, $i \neq m$, $m + 1$; $\varphi_m = \phi_m$, $\varphi_{m+1} = -\phi_m$, where $\phi_m = a_{m+\frac{1}{2}}\frac{[u]_\xi}{h^2}$.

Figure 4 shows the comparison between the analytical solution and the numerical solution of one-dimensional problem (4.8) at a set, fixed value of jump of the electric potential at the metal-plasma interface equal to $[u]_\xi = 2$ V and at the following values of problem parameters: $\rho_1 = 2.5 \times 10^{-5}\,\Omega\,\text{m}$, $\rho_2 = 3.33 \times 10^{-4}\,\Omega\,\text{m}$, $u_0 = -5$ V, $l = 0.01$ m and $\xi = 0.005$ m. Note here that, like in the case of scheme (4.4), difference scheme (4.10) is accurate in a class of piecewise constant coefficients. Figure 4 also shows the numerical solution of problem allowing for non-linear dependence (2.2) of the potential jump upon electric current density q, the functional form of which is given in [4], and the numerical values used are shown in Figure 5. Solution of the non-linear mesh problem was obtained by the iteration method, linear problem (4.10) being solved at each step of the iteration process.

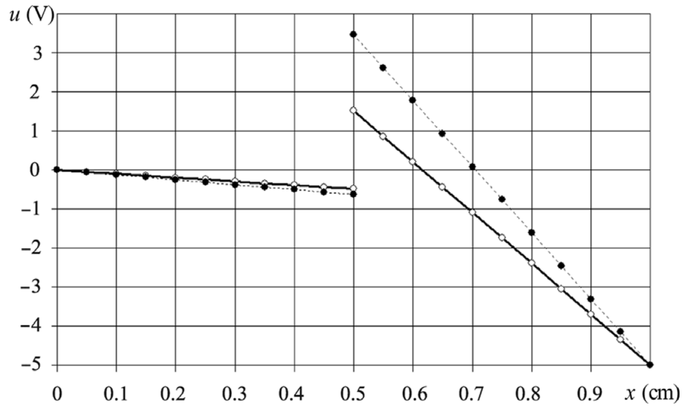

FIGURE 4. Distribution of potential in the ‘anode–arc plasma’ system (solid line shows an exact solution of the linear problem, open circles ∘ show the numerical solution of the linear problem, and solid circles • show the numerical solution of the non-linear problem).

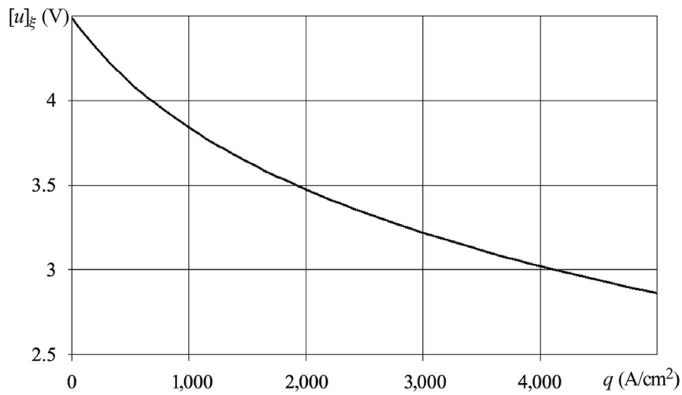

FIGURE 5. Anode potential drop versus electric current density, used for the solution of a non-linear problem (4.8).

In numerical modelling of physical processes occurring, for example, under conditions of arc welding of metals, the problem of distribution of the potential in the ‘anode–arc plasma’ system becomes multi-dimensional and requires allowance for a complex geometry of the interface between the conducting media. In particular, modeling of the current transfer process in the ‘electrode wire–electric arc plasma’ system in gas metal arc welding can be done on the basis of equations (3.10), which in the case of axial symmetry of the problem can be written down in the cylindrical coordinate system shown as in Figure 6 (it is taken into account in writing down equation (3.10) that $f \equiv 0$). This Figure also shows the boundary conditions used.

Results of numerical solution of the two-dimensional problem of distribution of the potential in the system under consideration, allowing for the non-linear dependence of the anode potential drop upon the current density at the anode (see Figure 5), are shown in Figure 7 in the form of isolines of the electric field potential.

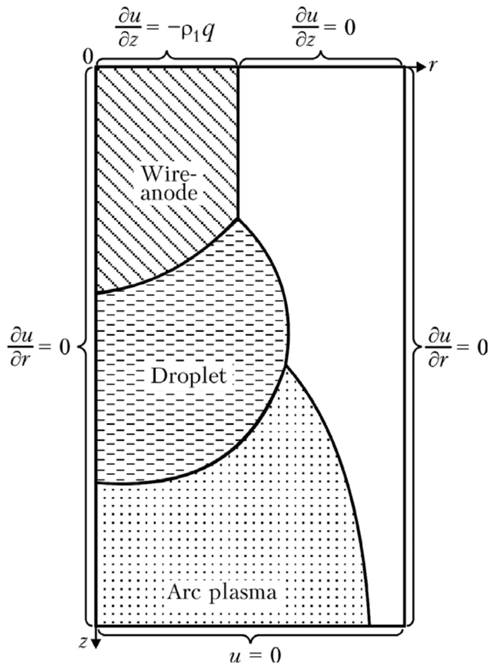

FIGURE 6. Schematic representation of ‘electrode wire–droplet–electric arc plasma’ system in gas metal arc welding.

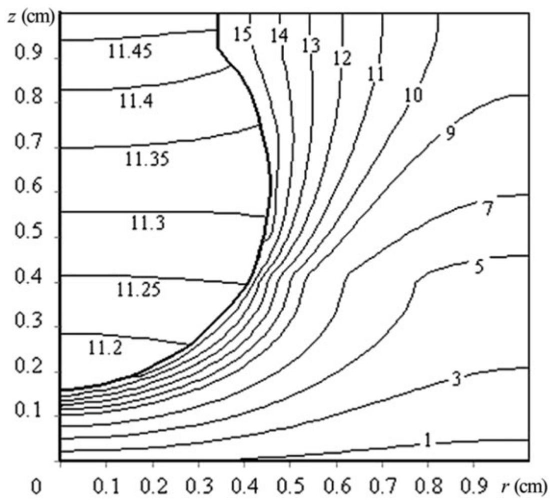

FIGURE 7. Field of potential in ‘electrode wire–droplet–electric arc plasma’ system in gas metal arc welding.

5 Conclusions and tasks for further investigations

The generalised problems of heat, mass and charge transfer in layered heterogeneous media with a discontinuous solution, which are suggested in this paper, are based on a physical natural description of the processes of transfer of a substance using a system of the

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first-order equations, one of which (scalar) is a law of conservation of substance, and the other (vector) is a generalised phenomenological law (Fick's, Fourier's, Darcy's or Ohm's law). The phenomenological law written down for the discontinuous potential in terms of specific resistances allows for the presence of the concentrated factors (e.g. concentrated resistance) at the interface between the media. It is this description that makes it possible to substantially widen the class of permissible input data for the problems of heat, mass and charge transfer, and, accordingly, the class of permissible solutions. For this purpose, space functions $W_2^{-1}(\Omega)$ with a negative metric can be regarded as elements of tensor Ξ in (3.8). By an initiative of the authors of this paper, Nomirovskii [9] considered the possibility of this generalisation and proved that at the said extention of the class of the coefficients of equations (3.8) there is also a unique solution to the problem in $L_2(\Omega)$. Extention of the class of permissible solutions is not only of a theoretical interest but is also important from the point of view of different physical applications. The transfer processes occurring in media with a finely dispersed and multiphase structure (e.g. in steels and alloys) and also in the anode sheath, where a metal contacts with plasma, are the objects that require such an extention. The generalised statement of the problem of charge transfer in form (3.10) is still to be proved to have unambiguous solvability in a class of functions $L_2(\Omega)$.

Distinctive feature of the suggested generalised statements is an end-to-end (homogeneous) description of the transfer processes in the entire multilayer system as a whole, without the use of explicit interface conditions at the boundary of discontinuity of a solution. This makes it possible to develop homogeneous calculation algorithms of the numerical solution (by the finite difference or finite element method). The efficiency and accuracy of difference schemes of the end-to-end computation developed on this basis was verified in this work on characteristic test problems having an exact solution.

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