A finite-difference scheme for the generalized diffuse interface model of the electrical breakdown process

A. S. Ponomarev[1], E. V. Zipunova[1]

[1]Keldysh Institute of Applied Mathematics, Moscow, Russia

The subject of the present work is numerical studies of a generalization of a diffuse interface model describing the development of the electrical breakdown channel. The Allen–Cahn type equation governing the phase field evolution is a nonlinear partial differential equation including 4-th order terms. The solutions of this equation may have singular behavior in some cases. In the paper, we propose a new finite-difference scheme allowing an exact accounting of the singularities of the solution and its accurate computation, even in the case when the boundary conditions are defined on objects of higher co-dimension.

Key words and phrases: diffuse interface model, phase field, stability, electrical breakdown.

1. Introduction

The electrical breakdown is a phenomenon of a sharp increase in the electric current in a dielectric medium under application of the electric field larger than a certain critical value. The process of the dielectric damage under the action of the electric field is complex and diverse: it can have various causes, mechanisms of development and accompanying physical processes [1].

Among the variety of mathematical models designed to describe the development of the electrical breakdown channel, we will highlight the diffuse interface type model proposed in the paper [2].

Diffuse interface type models are used to describe systems where a medium can exist in several different states — phases — separated by inter-phase boundaries. The spatial distribution of the phases is described by a smooth function ϕ — the phase field — with values close to a constant in each region of homogeneity. The inter-phase boundary is described as a thin separating layer, inside which the phase filed varies smoothly but fast. The thickness of the interface as well as the evolution of the phase field depend on the parameters of the model.

At present, diffuse interface models constitute a large class of approaches suitable for solving problems in various fields of science and technology. In particular, the model described in [2] itself is constructed as a formal generalization of previously known diffuse interface elastic fracture models. A study and further development of the mentioned model can be found in the papers [3, 4].

In the context of the electrical breakdown modelling, it is natural to consider two phases — the undamaged one, corresponding to the inital state of the medium before the breakdown process occurs; and the damaged one, corresponding to the state of the medium inside the breakdown channel. The particular feature of the breakdown process is that the damaged phase usually occupies an essentially one-dimensional spatial domain ("channel") in 3D space. In the work [3] it is shown that the original model proposed in [2] does not provide a correct mathematical setting in exclusive situations, thus certain modifications of the model are needed. These modifications lead to a strongly nonlinear and higher order partial differential equation governing the phase field evolution.

The subject of the present work is numerical studies of the generalization of the diffuse interface model describing the development of the electrical breakdown channel. The solutions of this equation may have singular behavior in some cases. We propose a new finite-difference scheme allowing an exact accounting of the singularities of the solution and its accurate computation for the problem under consideration. The scheme is suitable even for the cases where the boundary conditions are defined on objects of higher co-dimension. The presented scheme is based on finite volume approximations and uses specially chosen basis functions, accurately accounting the solution behavior at the boundaries. The possible types of singularities are analyzed as well.

2. The mathematical model

In this section, we give a short description of the phase field model for the electrical breakdown evolution suggested in [2]. A more extensive presentation of the model and a physical interpretation of its parameters are given in [3, 4].

Let $\Omega \subset \mathbb{R}^3$ be a bounded domain. The distribution of the damaged and undamaged phases is described by a smooth function $\phi = \phi(\mathbf{x}, t)$, $\phi: \Omega \times [0, +\infty)_t \to [0,1]$, called the phase field. The value $\phi = 1$ corresponds to the undamaged phase and the value $\phi = 0$ — to the damaged one.

The damaged and undamaged phases of the medium have different properties. The only one accounted in the simplest case is the electric permittivity ε, depending on the phase field and defined as:

$$\varepsilon(\mathbf{x}, t) = \varepsilon[\phi] = \frac{\varepsilon_0(\mathbf{x})}{f(\phi(\mathbf{x}, t)) + \delta}. \tag{1}$$

Here $\varepsilon_0(\mathbf{x})$ is the electric permittivity of the undamaged medium, $f(\phi) = 4\phi^3 - 3\phi^4$ is the so-called interpolation function, and $0 < \delta \ll 1$ is the regularization parameter, preventing form division by zero in (1). Such dependency of ε on ϕ assumes that the breakdown channel behaves like an ideal conductor with sufficiently large values of $\varepsilon \sim \varepsilon_0 / \delta$ in the damaged phase.

The electric field defined in the medium is described by the electric potential $\Phi = \Phi(\mathbf{x}, t)$, $\Phi: \Omega \times [0, +\infty)_t \to \mathbb{R}$.

The essence of the model is the following expression for the free energy of the medium:

$$\Pi = \int_\Omega \pi d\mathbf{x},$$

$$\pi = -\frac{1}{2}\varepsilon[\phi](\nabla\Phi, \nabla\Phi) + \Gamma\frac{1 - f(\phi)}{l^2} + \frac{\Gamma}{4}(\nabla\phi, \nabla\phi),$$

where $\Gamma > 0$, $l > 0$ are parameters of the model. The first term in π accounts for the energy of the electric field; the other terms account for the energy spent on the formation of the damaged medium. The special structure of these terms allows (i) to consider Γ as the energy needed to create a breakdown channel of unit length and (ii) to assign this energy to a spatial domain which is a cylinder of radius l with the center line being the breakdown channel. More details are given in [2].

Evolution of the fields ϕ and Φ is governed by the following equations:

$$\frac{\delta \Pi}{\delta \Phi} = 0; \quad \frac{1}{m}\frac{\partial \phi}{\partial t} = -\frac{\delta \Pi}{\delta \phi}.$$

Here $m > 0$ is the so-called mobility parameter. Speaking informally, these equations state that at each moment of time (i) the energy of the electric field Φ is minimized, whatever the distribution of the phase fields ϕ is, and (ii) the phase field ϕ evolves in a way minimizing the free energy of the system.

Computing the variational derivatives explicitly, one arrives to the following system of partial differential equations (here $(\cdot)' \equiv (\cdot)'_\phi$):

$$\mathrm{div}\big(\varepsilon[\phi]\nabla\Phi\big) = 0; \tag{2}$$

$$\frac{1}{m}\frac{\partial \phi}{\partial t} = \frac{1}{2}\varepsilon'(\phi)\big(\nabla\Phi, \nabla\Phi\big) + \frac{\Gamma}{l^2}f'(\phi) + \frac{1}{2}\Gamma\Delta\phi. \tag{3}$$

This system consists of two equations: the first one has the classical form of an equation for the electric potential, while the second one, governing the phase field evolution, is an Allen–Cahn type equation.

As it was discussed earlier, the nonlinear terms in π are responsible of the formation, during the damage evolution, of the "diffuse" breakdown channel, i.e., the "diffuse interface" itself. To study the structure of the diffuse interface, one usually considers a simplified problem. Its solution is a stationary distribution of the phase field in a neighbourhood of the damaged zone.

Therefore, we assume that $\Phi \equiv 0$ and equation (2) is satisfied identically hereinafter. In this case, the stationary solution of (3) satisfies

$$\frac{2}{l^2}f'(\phi) + \Delta\phi = 0. \tag{4}$$

Consider the spatial domain $\overline{\Omega} = [0, +\infty)_x \times I_y \times J_z$, where I and J are some intervals of $\mathbb{R}$.

Let the boundary conditions for (4) be defined as: $\phi|_{x=0} = 0$, $\phi \to 1$ as $x \to +\infty$, and also $\partial\phi/\partial\mathbf{n} = 0$ on the "faces" of $\overline{\Omega}$ perpendicular to the y- and z-axes. The symbol $\partial/\partial\mathbf{n}$ denotes the derivative along the external unit normal $\mathbf{n}$ to $\partial\Omega$. With such boundary conditions being defined, it is easy to see that the solution of (4) depends only on x, i.e., $\phi(\mathbf{x}) = \phi(x)$.

Thus, equation (4) reduces to:

$$\frac{\partial^2 \phi}{\partial x^2} = -\frac{2}{l^2}f'(\phi),$$

which further can be simplified to the equation

$$\frac{\partial \phi}{\partial x} = \frac{2}{l}\sqrt{1 - f(\phi)}, \tag{5}$$

accompanied by the boundary condition $\phi(0) = 0$. It can be shown that the solution of this problem exists and is unique.

So, we find the distribution of the phase field ϕ in the neighbourhood of the plane boundary located at $x = 0$. At $x = 0$ we have $\phi = 0$ corresponding to the completely damaged phase. It can be shown [3] that for $x > l$ the solution of the problem $\phi \approx 1$. In other words, the damaged medium is

localized in the vicinity of $x = 0$. Thus, ϕ properly describes the damaged medium in the neighbourhood of a completely damaged plane. This is exactly the prototypical behavior of the phase field distribution governed by the nonlinear terms in π.

Such analysis is suitable in the case if one assumes that the breakdown channel is a plane (i.e., not a "breakdown channel" but rather a "breakdown fracture"). In more realistic setting one expects ϕ to be a solution of (4) localized around a 1D line, or a curve, embedded into the 3D domain $\bar{\Omega}$.

In other words, it is natural to consider the following setting. Let, again, $\Phi \equiv 0$. Consider equation (4) in the domain $\bar{\Omega} = \mathbb{R}_x \times \mathbb{R}_y \times J_z$ with J being some interval, together with the boundary conditions: $\phi|_{x,y=0} = 0$, $\phi \to 1$ as $r = \sqrt{x^2 + y^2} \to +\infty$, and $\partial\phi / \partial\mathbf{n} = 0$ at the faces of $\bar{\Omega}$ perpendicular to the z-axis.

In this case, we have a boundary value problem for equation (4) considered in a three-dimensional domain with boundary conditions defined on a co-dimension 2 "boundary", which is a straight line $x = y = 0$. It can be shown that such problem statement is not correct because a 2nd order partial differential equation (4) does not allow the definition of boundary conditions on co-dimension 2 boundaries. The reasons are explained in details in the paper [3].

A modification of the problem guaranteeing the correctness in the case when the boundary conditions are defined at an object of co-dimension 2 is given in [3]. It is based on the of specially chosen higher-order differential terms addition into the expression for the free energy π. Then, the proposed expression for π is:

$$\pi = -\frac{1}{2}\varepsilon[\phi](\nabla\Phi, \nabla\Phi) + \Gamma\frac{1-f(\phi)}{l^2} + \frac{\Gamma}{4}(\nabla\phi, \nabla\phi) + \alpha\frac{\Gamma l^2}{8}(\Delta\phi)^2 + \beta\frac{1}{p}\Gamma l^{p-2}\|\nabla\phi\|_2^p. \quad (6)$$

Here $\alpha, \beta \geqslant 0$ are parameters, $p \geqslant 4$ is an even natural number. The differential operator $\mathrm{div}\left(\|\nabla\phi\|_2^{p-2}\nabla\phi\right)$ is usually called the p-laplacian, and $\Delta^2\phi = \Delta(\Delta\phi)$ is the bi-harmonic operator. For simplicity hereinafter we set $p = 4$.

Since we will consider only the phase field equation later, we assume that $\Phi \equiv 0$ in (2), (3). Then the resulting equation for ϕ is:

$$\frac{1}{m}\frac{\partial\phi}{\partial t} = \frac{\Gamma}{l^2}f'(\phi) + \frac{1}{2}\Gamma\Delta\phi - \alpha\frac{\Gamma l^2}{4}\Delta^2\phi + \beta\Gamma l^{p-2}\,\mathrm{div}\left(\|\nabla\phi\|_2^{p-2}\nabla\phi\right), \quad (7)$$

or, in a more compact form,

$$\frac{1}{m}\frac{\partial\phi}{\partial t} = \frac{\Gamma}{l^2}f'(\phi) + \Gamma\,\mathrm{div}\,\boldsymbol{\rho}, \quad (8)$$

where

$$\boldsymbol{\rho} = \frac{1}{2}\nabla\phi - \alpha\frac{l^2}{4}\nabla(\Delta\phi) + \beta l^2\|\nabla\phi\|_2^2\nabla\phi. \quad (9)$$

3. The finite-difference scheme
3.1. General setting
Our goal is to study stationary solutions of (8) numerically, and we are mostly interested in

three particular cases: two of them are described in section 2 and the third one is described below. All the three cases can be called one-dimensional, meaning that each one has only one significant spatial variable r, as explained below. The cases only differ in boundary conditions, defined on boundaries of different co-dimension:

1. $\bar{\Omega} = [0, +\infty)_x \times I_y \times J_z$, $r \equiv x$, $\phi|_{x=0} = 0$, $\phi \rightarrow 1$ at $r \equiv x \rightarrow +\infty$. This is the planar case. The boundary condition is given on a co-dimension 1 set — the 2D plane $r \equiv x = 0$.

2. $\bar{\Omega} = \mathbb{R}_x \times \mathbb{R}_y \times J_z$, $\phi|_{x,y=0} = 0$, $\phi \rightarrow 1$ at $r = \sqrt{x^2 + y^2} \rightarrow +\infty$. This is the axially symmetric case. The boundary condition is given on a co-dimension 2 set — the 1D axis $r = 0$.

3. $\bar{\Omega} = \mathbb{R}_x \times \mathbb{R}_y \times \mathbb{R}_z$, $\phi|_{x,y,z=0} = 0$, $\phi \rightarrow 1$ at $r = \sqrt{x^2 + y^2 + z^2} \rightarrow +\infty$. This is the spherically symmetric case. The boundary condition is given on a co-dimension 3 set — the 0D point $r = 0$.

Note that the only difference between the cases is the dimension of the set where the boundary condition is defined.

Cases 1 and 2 were discussed in section 2. Case 3 naturally extends cases 1 and 2.

According to the derivation of the equations, stationary solutions minimize the free energy Π. In turn, the evolutionary equations of the model are constructed to minimize Π during temporal evolution (see section 2 for details). Therefore, it is possible to construct the stationary solution by solving the evolutionary equations on a sufficiently long time interval: the resulting limit solution will be the stationary solution of the equations under consideration.

In cases 2 and 3 it is natural to use cylindrical and spherical coordinate systems, respectively, and assume that the phase field depends only on the radial variable, i.e., $\phi = \phi(r,t)$. So, in each setting we have $\phi(\mathbf{x},t) = \phi(r,t)$.

Since we assume that the solutions decay quite fast to the their values at infinity, we shift the boundary condition from infinity to a finite point $r = R$ with a sufficiently large value of R. Then, the boundary condition for all three cases can be written as $\phi(0) = 0$ $\phi(R) = 1$ with $R \gg l$ being the external radius of $\bar{\Omega}$.

To construct the finite-dimensional problem, we use the finite volume technique.

To proceed, decompose $\bar{\Omega}$ into $n+1$ cells (planar, or cylindrical, or spherical layers), which we refer to as $\Omega_0, \ldots, \Omega_n$. Let the boundaries of the cells be $0 = r_{-1/2}, r_{1/2}, \ldots, r_{n+1/2} = R$.

Define $V(r)$ a volume of planar, cylindrical or spherical subdomain of $\bar{\Omega}$ extended from 0 to r. Let $S(r)$ be the area of its (external) boundary. Then, the volume of the cell Ω_i is equal to $dV_i = V(r_{i+1/2}) - V(r_{i-1/2})$, and areas of its internal and external boundaries are given by $S_{i-1/2} = S(r_{i-1/2})$ and $S_{i+1/2} = S(r_{i+1/2})$, respectively. For the cases under consideration one has:

1. The planar case. $V(r) = r \cdot |I_y| \cdot |J_z|$, $S(r) = |I_y| \cdot |J_z|$. Since the coefficients not depending on r can be cancelled during the construction of the finite-difference scheme (see below), we just establish $V(r) = r$, $S(r) = 1$.

2. The axisymmetric case. $V(r) = \pi r^2 \cdot |J_z|$, $S(r) = 2\pi r \cdot |J_z|$. On the same basis as before,

we set $V(r) = r^2$, $S(r) = 2r$.

3. The sperically symmetric case. $V(r) = (4/3)\pi r^3$, $S(r) = 4\pi r^2$, or, again, $V(r) = r^3$, $S(r) = 3r^2$.

Note that for each of the three cases we can set $V(r) = r^{k+1}$, $S(r) = (k+1)r^k$, where $k = 0$ for the planar case, $k = 1$ for the axisymmetric case and $k = 2$ for the sperically symmetric one.

We now proceed to the construction of the finite-volume scheme. First, integrate (8) over $\left[t_j, t_{j+1}\right] \times \Omega_i$. For the left-hand side, one has:

$$\int_{\Omega_i} \int_{t_j}^{t_{j+1}} \frac{1}{m} \frac{\partial \phi}{\partial t} dt d\mathbf{x} = \frac{1}{m} \int_{\Omega_i} \left[\phi(\mathbf{x}, t_{j+1}) - \phi(\mathbf{x}, t_j)\right] d\mathbf{x} = \frac{dV_i}{m} \left[\tilde{\phi}_i(t_{j+1}) - \tilde{\phi}_i(t_j)\right],$$

where $\tilde{\phi}_i$ is the integral average of ϕ over Ω_i. For the right-hand side one obtains:

$$\int_{t_j}^{t_{j+1}} \int_{\Omega_i} \left(\frac{\Gamma}{l^2} f'(\phi) + \Gamma \operatorname{div} \boldsymbol{\rho}\right) d\mathbf{x} dt = \Gamma \int_{t_j}^{t_{j+1}} \left(\frac{1}{l^2} \int_{\Omega_i} f'(\phi) d\mathbf{x} + \int_{\partial \Omega_i} (\boldsymbol{\rho}, \mathbf{n}) dS\right) dt.$$

Since ϕ depends only on r, the flux density $\boldsymbol{\rho}$ is always collinear to the r-axis and we have:

$$\int_{\partial \Omega_i} (\boldsymbol{\rho}, \mathbf{n}) dS = F_{i+1/2} - F_{i-1/2} = \rho_{i+1/2} S_{i+1/2} - \rho_{i-1/2} S_{i-1/2},$$

where

$$F_{i\pm1/2}(t) = \int_{r=r_{i\pm1/2}} (\boldsymbol{\rho}, \mathbf{n}) dS = \int_{r=r_{i\pm1/2}} \rho_r dS = \rho_r S(r_{i\pm1/2}) = \rho_{i\pm1/2}(t) \cdot S_{i\pm1/2}.$$

Here ρ_r defines the only nonvanishing radial component of $\boldsymbol{\rho}$ and $\rho_{i\pm1/2}(t) = \rho_r(r_{i\pm1/2}, t)$ is the flux density over the respective boundary.

Hence, the balance equation for the cell Ω_i is:

$$\frac{dV_i}{m} \left[\tilde{\phi}_i(t_{j+1}) - \tilde{\phi}_i(t_j)\right] = \Gamma \int_{t_j}^{t_{j+1}} \left[\frac{1}{l^2} \int_{\Omega_i} f'(\phi) d\mathbf{x} + \rho_{i+1/2} S_{i+1/2} - \rho_{i-1/2} S_{i-1/2}\right] dt. \tag{10}$$

The scheme in its final form will be presented later. Here we just mention that the first term under the integral in the right-hand side of (10) can be approximated as $l^{-2} \cdot dV_i \cdot f'\left[\tilde{\phi}_i(t_j)\right]$ and the time integral can be approximated in the simplest way as a product of $(t_{j+1} - t_j)$ and the integrand, evaluated at t_j.

A more difficult task to which we proceed now is to construct approximations $\rho_{i\pm1/2}$ of the flux density $\boldsymbol{\rho}$.

First, note that for an arbitrary function $\psi(\mathbf{x}) = \psi(r)$, we have:

$$(\nabla \psi)_r = \frac{\partial \psi}{\partial r}, \quad (\nabla \psi)_\theta = (\nabla \psi)_z = 0,$$

where $\nabla \psi$ also only depends on r. Therefore, from (9) we arrive to:

$$\rho_r = \frac{1}{2}\frac{\partial \phi}{\partial r} - \alpha \frac{l^2}{4}\frac{\partial}{\partial r}(\Delta\phi) + \beta l^2 \left(\frac{\partial \phi}{\partial r}\right)^3. \tag{11}$$

Conventionally, the finite-volume method, in its simplest form, assumes that the finite-dimensional solution is a constant function inside every finite volume. Since in our problem the solution can be finite but singular or fast growing function at $r = 0$, where the boundary condition is defined on a lower dimensional set, such an assumption can be unreasonable. To account the probably singular solution behaviour, we assume that the solution can be described well using a linear combination of two specially chosen basis functions. Their concrete form differs for cases 1 to 3 mentioned above and is a subject of special analysis performed later. Below we assume that the basis functions are known and show a general construction of the scheme.

So, let us construct the approximation of some function $\psi(r)$ in the neighbouring finite volume cells Ω_i and Ω_{i+1}, if average values $\tilde{\psi}_i$ and $\tilde{\psi}_{i+1}$ over Ω_i and Ω_{i+1} are known.

Let

$$g(r) = a \cdot g^{(a)}(r) + b \cdot g^{(b)}(r) \tag{12}$$

be the function constructed as a linear combination of two basis functions $g^{(a)}$ and $g^{(b)}$ (which are for local approximation of ψ) with a and b being the respective weights. The condition to determine a and b in such a way that the integral averages of $g(r)$ over Ω_i and Ω_{i+1} are equal to the given values of $\tilde{\psi}_i$, $\tilde{\psi}_{i+1}$, respectively, is given by

$$\int_{r_{i-1/2}}^{r_{i+1/2}} \left[\tilde{\psi}_i - g(r)\right]S(r)dr = 0; \qquad \int_{r_{i+1/2}}^{r_{i+3/2}} \left[\tilde{\psi}_{i+1} - g(r)\right]S(r)dr = 0. \tag{13}$$

Let

$$\int_{r_{i-1/2}}^{r_{i+1/2}} g^{(a)}(r)S(r)dr = I_i^{(a)}; \qquad \int_{r_{i-1/2}}^{r_{i+1/2}} g^{(b)}(r)S(r)dr = I_i^{(b)}.$$

Since $g^{(a)}$, $g^{(b)}$ are known, the values of $I_i^{(a)}$ and $I_i^{(b)}$ are assumed to be known as well. System (13) is equivalent to

$$aI_i^{(a)} + bI_i^{(b)} = \left(r_{i+1/2}^{k+1} - r_{i-1/2}^{k+1}\right)\tilde{\psi}_i; \qquad aI_{i+1}^{(a)} + bI_{i+1}^{(b)} = \left(r_{i+3/2}^{k+1} - r_{i+1/2}^{k+1}\right)\tilde{\psi}_{i+1},$$

which has the solution

$$a = \frac{\left(r_{i+1/2}^{k+1} - r_{i-1/2}^{k+1}\right)I_{i+1}^{(b)}}{\Delta}\cdot\tilde{\psi}_i + \frac{-\left(r_{i+3/2}^{k+1} - r_{i+1/2}^{k+1}\right)I_i^{(b)}}{\Delta}\cdot\tilde{\psi}_{i+1}; \tag{14}$$

$$b = \frac{-\left(r_{i+1/2}^{k+1} - r_{i-1/2}^{k+1}\right)I_{i+1}^{(a)}}{\Delta}\cdot\tilde{\psi}_i + \frac{\left(r_{i+3/2}^{k+1} - r_{i+1/2}^{k+1}\right)I_i^{(a)}}{\Delta}\cdot\tilde{\psi}_{i+1}; \tag{15}$$

where $\Delta = I_i^{(a)}I_{i+1}^{(b)} - I_i^{(b)}I_{i+1}^{(a)}$.

Expressions (14) and (15) allow to compute the coefficients a and b as soon as $\tilde{\psi}_i$ and $\tilde{\psi}_{i+1}$ are given and $I_i^{(a,b)}$ are pre-computed.

The derivative $\partial\psi/\partial r$ at the boundary $r_{i+1/2}$ between the cells Ω_i and Ω_{i+1} can be

approximated using (12) as:

$$\left[\frac{\partial \psi}{\partial r}\right]_{i+1/2} = g'(r_{i+1/2}) = a \cdot \left(g^{(a)}\right)'(r_{i+1/2}) + b \cdot \left(g^{(b)}\right)'(r_{i+1/2}).$$

We assume here that the derivatives $\left(g^{(a)}\right)'$ and $\left(g^{(b)}\right)'$ are known.

To define the approximation of $\partial\phi/\partial r$ at the inter-cell boundaries with $r_{3/2},\ldots,r_{n-1/2}$ — i.e., at all the inter-cell boundaries except the first two and the last one, we set $\tilde{\psi} = \tilde{\phi}$ and define $g^{(a)}(r) = r$, $g^{(b)}(r) = 1$. In this case $g' \equiv a$; computation of $I^{(a)}$ and $I^{(b)}$ also does not present any difficulties. That is, we approximate ϕ with a linear function in pairs of neighbouring cells.

The approximation of $\partial\phi/\partial r$ in the boundary cells of Ω is a more complicated task, which will be addressed in the following section.

Finally, we need to approximate $\Delta\phi$ and its derivative with respect to r (see (11)). Proceeding in the same way as above, we arrive to:

$$dV_i \cdot \tilde{\Delta\phi}_i = \frac{\partial\phi}{\partial r}(r_{i+1/2}) \cdot S_{i+1/2} - \frac{\partial\phi}{\partial r}(r_{i-1/2}) \cdot S_{i-1/2}. \tag{16}$$

With $\tilde{\Delta\phi}_i$ being defined, the approximation of $\partial(\Delta\phi)/\partial r$ at the boundaries $r_{1/2},\ldots,r_{n-1/2}$ (i.e., at all the internal boundaries) can be constructed in the same way as it was done for $\partial\phi/\partial r$, with $\tilde{\psi} = \tilde{\Delta\phi}$, $g^{(a)}(r) = r$, $g^{(b)}(r) = 1$.

3.2. Approximation of the boundary conditions

We now turn to the most essential part of the paper — the approximation of the boundary conditions for equation (8), (9) at $r = 0$.

The boundary conditions for (8), (9), discussed in the previous section, are defined as: $\phi(0) = 0$, $\phi(R) = 1$, where $R > 0$ and $R/l \gg 1$. If the coefficient $\alpha \neq 0$ in (7), these conditions are not enough due to higher order of the differential operator involved (the equation is of the 2nd order for $\alpha = 0$ and of the 4th order for $\alpha \neq 0$). One option to define the additional boundary conditions is to set

$$\frac{\partial\phi}{\partial r}\Big|_{r=0} = 0, \qquad \Delta\phi\big|_{r=R} = 0.$$

In the discreet setting, the boundary condition at $r = R$ is easily defined as $\tilde{\phi}_n = 1$, $\tilde{\Delta\phi}_n = 0$. This turns out to be sufficient as at $R \gg l$ the solution ϕ of (8), (9) is smooth, slowly varying and almost equal to 1.

A much more complex situation arises at $r = 0$. The reason is twofold: first, the spatial differential operator in (8) has a geometric singularity at $r = 0$ in cylindrical and spherical coordinates; second, at least for the axisymmetric and spherically symmetric cases it is expected that ϕ and $\Delta\phi$ may grow fast or even have a singularity at $r = 0$.

The approach suggested further assumes that these singularities, if any, can be approximated

with high accuracy using specially chosen basis functions $g^{(a,b)}$.

So, to define the boundary condition at $r = 0$, we proceed as follows.

Let us choose such functions $g^{(a)}$ and $g^{(b)}$ that: (i) both of them satisfy the boundary condition at $r = 0$ and (ii) one of them has the same asymptotic behavior at $r = 0$ as it is expected for ϕ. Then, using $g(r)$ defined above, it is easy to obtain the desired approximation:

$$\left[\frac{\partial \phi}{\partial r}\right]_{-1/2} = g'(0); \qquad \left[\frac{\partial \phi}{\partial r}\right]_{1/2} = g'(r_{1/2});$$

$$\left[\frac{\partial (\Delta \phi)}{\partial r}\right]_{-1/2} = \frac{\partial}{\partial r}\left[r^k \frac{\partial}{\partial r}\left(\frac{1}{r^k}\frac{\partial g}{\partial r}\right)\right]\bigg|_{r=0}.$$

In the last expression, we use the general formula for the Laplacian of $g = g(r)$ for the planar, axisymmetric and spherically symmetric cases:

$$\Delta g = \frac{1}{r^k}\frac{\partial}{\partial r}\left(r^k \frac{\partial g}{\partial r}\right). \tag{17}$$

We now need to define concrete basis functions to approximate ϕ in first two cells of the mesh depending on concrete setting and values of α and β.

The planar case.

In this case, we do not expect any singularities in ϕ (and also in $\Delta \phi$, if $\alpha \neq 0$) at $r = 0$. The motivation is as follows. One has $S(0) = 1 \neq 0$. Hence, for the flux $F_{-1/2}$ to be nonvanishing it is enough to have a nonvanishing and bounded flux density $\rho_{-1/2}$. For $\alpha = 0$, the only boundary condition at $r = 0$ is $\phi(0) = 0$. So, it is possible to define $g^{(a)} = r^2$, $g^{(b)} = r$. For $\alpha \neq 0$ one also has the boundary condition $\partial \phi / \partial r |_{r=0} = 0$ and one can set $g^{(a)} = r^3$, $g^{(b)} = r^2$.

The axisymmetric case.

One has $S(0) = 0$, and, hence, $F_{-1/2} = 0$ as soon as the flux density ρ_r is bounded. However, if we assume that $\rho_r \sim 1/r$ then $\rho_r(r)S(r) \to 2$ as $r \to +0$, i.e., the flux is bounded and nonvanishing. If ρ_r grows asymptotically slower than $1/r$ then the flux is equal to zero, otherwise it is unbounded.

Let now $\alpha = \beta = 0$. Then, in expression (11) we have $\rho_r \sim \partial \phi / \partial r$ and try to define $g^{(a)}$ such that $\left(g^{(a)}\right)' = C_0 / r$. After integration we have $g^{(a)} = C_0 \ln r + C_1$ and $g^{(a)} \to \infty$ as $r \to +0$. Hence, the boundary condition $g^{(a)}(0) = 0$ can not be satisfied. This indirectly confirms the conclusions from [3] that for the considered values of parameters the solution of (8) does not exist.

Let $\alpha = 0$, $\beta \neq 0$. Then (11) includes the term $\partial \phi / \partial r$ in the power of 1 and 3. Hence, one can assume $\left(g^{(a)}\right)' = C_0 r^{-1/3}$. The first degree of the derivative gives a vanishing input into the flux; the input from the third derivative is finite and nonvanishing. As a result, after integration

$g^{(a)} = C_0 \cdot (3/2) \cdot r^{2/3} + C_1$. Taking the boundary condition into account, define $g^{(a)} = r^{2/3}$. The second basis function can be defined as $g^{(b)} = r$.

Let $\alpha \neq 0$, $\beta = 0$ or $\beta \neq 0$. Then, (11) includes the $\partial(\Delta\phi)/\partial r$ term (it also includes $\partial\phi/\partial r$ term, but the latter one is vanishing due to the boundary condition). So, one needs to find $g^{(a)}$ such that $\partial\left(\Delta g^{(a)}\right)/\partial r = C_0/r$. Note that the Laplacian of $g^{(a)} = g^{(a)}(r)$ in axisymmetric case is given by (17) with $k = 1$. Integrating $\partial\left(\Delta g^{(a)}\right)/\partial r$ three times, we arrive to $g^{(a)} = (C_0/4)r^2(\ln r - 1) + C_1 r^2/4 + C_2 \ln r + C_3$. To satisfy the boundary conditions, one need $g^{(a)}(0) = 0$, therefore $C_2 = C_3 = 0$, and it is enough to set $g^{(a)} = r^2 \ln r$. So, the function $g^{(a)}$ satisfies the boundary condition $\left(g^{(a)}\right)'(0) = 0$. The second basis function can be chosen as $g^{(b)} = r^2$.

The spherically symmetric case.
Similarly to the axisymmetric case, we are about to find such a basis function that the flux $F_{-1/2}$ would be finite and nonvanishing. Then, ρ_r should have a singularity of form $1/r^2$ since in this case $\rho_r(r)S(r) \to 3$ as $r \to +0$.

Let $\alpha = \beta = 0$. Define $g^{(a)}$ such that $\left(g^{(a)}\right)' = C_0/r^2$. After integration, one has $g^{(a)} = -C_0/r + C_1$. We see that $g^{(a)} \to \infty$ as $r \to +0$, — i.e., the boundary condition $g^{(a)}(0) = 0$ can not be satisfied.

Let $\alpha = 0$, $\beta \neq 0$. Similarly to the previous case, one needs $\left(g^{(a)}\right)' = C_0 r^{-2/3}$, and, hence, $g^{(a)} = C_0 \cdot 3 \cdot r^{1/3} + C_1$. Taking the boundary condition into account, we finally define $g^{(a)} = r^{1/3}$, $g^{(b)} = r$.

Now let $\alpha \neq 0$, $\beta = 0$ or $\beta \neq 0$. Repeating the previous argumentation, we get $\partial\left(\Delta g^{(a)}\right)/\partial r = C_0/r^2$, and, after integration, $\left(g^{(a)}\right)' = -C_0/2 + C_1 r/3 + C_2/r^2$ where $C_0 \neq 0$. As a result, $\left(g^{(a)}\right)'(0) \neq 0$ and the boundary condition for derivative can not be satisfied.

So, we arrive to the situation when in the spherically symmetric case it looks impossible to satisfy the desired boundary conditions both for $\alpha = \beta = 0$ and for $\alpha \neq 0$.

3.3. The finite-difference scheme
In this section, we present the derived finite difference scheme in a closed form together with the approximations of the boundary conditions. In previous subsections, it was assumed that the radial coordinates of the cell boundaries can be an arbitrary monotonically increasing sequence $0 = r_{-1/2}, r_{1/2}, \ldots, r_{n-1/2}, r_{n+1/2} = R$. Hereinafter we assume, for simplicity, that the spatial mesh is uniform with a step h: $r_{i-1/2} = ih$. We also assume that the temporal step size is constant, i.e., $t_j = j\tau$ with a

fixed τ. The values of mesh functions defined at a time t_j will be denoted by a superscript j.

The initial condition is given by the cell averages $\tilde{\phi}_i^0$, $i = \overline{0,n}$. In the finite-difference equation below, $k = 0$ corresponds to the planar case, $k = 1$ to the axisymmetric case and $k = 2$ to the spherically symmetric one.

Based on the derivation of the previous section, the complete finite-difference scheme for sovling equation (8), (9) is as follows.

$$\frac{1}{m}\left(\tilde{\phi}_i^{j+1} - \tilde{\phi}_i^j\right) = \tau\frac{\Gamma}{l^2} f'\left(\tilde{\phi}_i^j\right) + \frac{\tau}{dV_i}\Gamma\left(\rho_{i+1/2}^j S_{i+1/2} - \rho_{i-1/2}^j S_{i-1/2}\right) \text{ for } i = \overline{0,n-1};$$

$$\tilde{\phi}_n^j = 1;$$

(18)

$$dV_i = \left(r_{i+1/2}\right)^{k+1} - \left(r_{i-1/2}\right)^{k+1}; \qquad S_{i\pm1/2} = (k+1)\left(r_{i\pm1/2}\right)^k;$$

$$\rho_{i\pm1/2}^j = \frac{1}{2}\left[\frac{\partial\phi}{\partial r}\right]_{i\pm1/2}^j - \alpha\frac{l^2}{4}\left[\frac{\partial(\Delta\phi)}{\partial r}\right]_{i\pm1/2}^j + \beta l^2\left(\left[\frac{\partial\phi}{\partial r}\right]_{i\pm1/2}^j\right)^3;$$

(19)

$$\left[\frac{\partial\phi}{\partial r}\right]_{i+1/2}^j = a_{i+1/2}^j \text{ for } i = \overline{1,n-1};$$

(20)

$$\{\tilde{\phi}_i^j\}_{i=1}^n \hat{I}\{a_{i+1/2}^j\}_{i=1}^{n-1}, \text{ where } g^{(a)} = r,\ g^{(b)} = 1;$$

$$\tilde{\Delta\phi}_i^j = \frac{1}{dV_i}\left(\left[\frac{\partial\phi}{\partial r}\right]_{i+1/2}^j S_{i+1/2} - \left[\frac{\partial\phi}{\partial r}\right]_{i-1/2}^j S_{i-1/2}\right) \text{ for } i = \overline{0,n-1};$$

$$\tilde{\Delta\phi}_n^j = 0;$$

(21)

$$\left[\frac{\partial(\Delta\phi)}{\partial r}\right]_{i+1/2}^j = c_{i+1/2}^j \text{ for } i = \overline{0,n-1};$$

(22)

$$\{\tilde{\Delta\phi}_i^j\}_{i=0}^n \hat{I}\{c_{i+1/2}^j\}_{i=0}^{n-1}, \text{ where } g^{(c)} = r,\ g^{(d)} = 1;$$

$$\left[\frac{\partial\phi}{\partial r}\right]_{i-1/2}^j = a_{1/2}^j\left(g_{1/2}^{(a)}\right)'(r_{i-1/2}) + b_{1/2}^j\left(g_{1/2}^{(b)}\right)'(r_{i-1/2}) \text{ for } i = \overline{0,1};$$

(23)

$$\left[\frac{\partial(\Delta\phi)}{\partial r}\right]_{-1/2}^j = a_{1/2}^j\left.\frac{\partial(\Delta g^{(a)})}{\partial r}\right|_{r=0} + b_{1/2}^j\left.\frac{\partial(\Delta g^{(b)})}{\partial r}\right|_{r=0};$$

(24)

$$\left\{\tilde{\phi}_0^j, \tilde{\phi}_1^j\right\}\hat{I}\left\{a_{1/2}^j, b_{1/2}^j\right\}, \text{ where } g_{1/2}^{(a)},\ g_{1/2}^{(b)} \text{ are defined below.}$$

In the equations above, the symbol "$\hat{I}$" denotes the application of the reconstruction procedure mapping the cell averages to the coefficients of the expansion in the basis functions $g^{(a)}$ and $g^{(b)}$, see equations (14) and (15).

The concrete form of the basis functions $g^{(a)}$ and $g^{(b)}$ depends on the symmetry properties of the problem setting and the values of the coefficients α and β:

1. The planar case, $\alpha = 0$:

$$g_{1/2}^{(a)} = r^2, \quad \left(g_{1/2}^{(a)}\right)' = 2r, \quad I^{(a)} = \left.\frac{1}{3}r^3\right|_{r_\xi}^{r_\eta};$$

$$g_{1/2}^{(b)} = r, \quad \left(g_{1/2}^{(b)}\right)' = 1, \quad I^{(b)} = \left.\frac{1}{2}r^2\right|_{r_\xi}^{r_\eta}.$$

2. The planar case, $\alpha \neq 0$:

$$g_{1/2}^{(a)} = r^3, \quad \left(g_{1/2}^{(a)}\right)' = 3r^2, \quad \frac{\partial\left(\Delta g_{1/2}^{(a)}\right)}{\partial r} = 6, \quad I^{(a)} = \left.\frac{1}{4}r^4\right|_{r_\xi}^{r_\eta};$$

$$g_{1/2}^{(b)} = r^2, \quad \left(g_{1/2}^{(b)}\right)' = 2r, \quad \frac{\partial\left(\Delta g_{1/2}^{(b)}\right)}{\partial r} = 0, \quad I^{(b)} = \left.\frac{1}{3}r^3\right|_{r_\xi}^{r_\eta}.$$

3. The axisymmetric case, $\alpha = 0$, $\beta \neq 0$:

$$g_{1/2}^{(a)} = r^{2/3}, \quad \left(g_{1/2}^{(a)}\right)' = \frac{2}{3}r^{-1/3}, \quad I^{(a)} = \left.\frac{3}{4}r^{8/3}\right|_{r_\xi}^{r_\eta};$$

$$g_{1/2}^{(b)} = r, \quad \left(g_{1/2}^{(b)}\right)' = 1, \quad I^{(b)} = \left.\frac{2}{3}r^3\right|_{r_\xi}^{r_\eta};$$

$$\rho_{-1/2}^j S_{-1/2} = \frac{16}{27}(a_{1/2}^j)^3.$$

4. The axisymmetric case, $\alpha \neq 0$:

$$g_{1/2}^{(a)} = r^2 \ln r, \quad \left(g_{1/2}^{(a)}\right)' = r(2\ln r + 1), \quad \frac{\partial\left(\Delta g_{1/2}^{(a)}\right)}{\partial r} = \frac{4}{r}, \quad I^{(a)} = \left.\frac{1}{8}r^4(4\ln r - 1)\right|_{r_\xi}^{r_\eta};$$

$$g_{1/2}^{(b)} = r^2, \quad \left(g_{1/2}^{(b)}\right)' = 2r, \quad \frac{\partial\left(\Delta g_{1/2}^{(a)}\right)}{\partial r} = 0, \quad I^{(b)} = \left.\frac{1}{2}r^4\right|_{r_\xi}^{r_\eta};$$

$$\rho_{-1/2}^j S_{-1/2} = 8a_{1/2}^j.$$

5. The spherically symmetric case, $\alpha = 0$, $\beta \neq 0$:

$$g_{1/2}^{(a)} = r^{1/3}, \quad \left(g_{1/2}^{(a)}\right)' = \frac{1}{3}r^{-2/3}, \quad I^{(a)} = \left.\frac{9}{10}r^{10/3}\right|_{r_\xi}^{r_\eta};$$

$$g_{1/2}^{(b)} = r, \quad \left(g_{1/2}^{(b)}\right)' = 1, \quad I^{(b)} = \left.\frac{3}{4}r^4\right|_{r_\xi}^{r_\eta};$$

$$\rho_{-1/2}^j S_{-1/2} = \frac{1}{9}(a_{1/2}^j)^3.$$

In the equations above, $r_{\xi,\eta}$ denote generic integration limits.

4. Numerical experiment

In this section, we show examples of application of the proposed finite-difference scheme (18) – (24) for solving equation (7), (8).

Let the parameters of the model be defined as:
$$l = 1.0, \ \ \Gamma = 1.0, \ \ m = 0.5.$$

The external radius $R = 5$. As it will be seen, such value is enough to provide correct asymptotic behavior of ϕ at large values of $r \gg l$.

Let $n = 300$ for $\alpha = 0$ and $n = 150$ otherwise. Then, the spatial mesh step size is $h = 1/60 \approx 0.0167$ or $h = 1/30 \approx 0.0333$, respectively. The time step is $\tau = 5 \cdot 10^{-7}$.

Since we are interested in the limit solution for $t \to +\infty$, the choice of the initial conditions is not important. In the presented simulations it was set $\tilde{\phi}_i^0 = \sin\left[(h/2 + ih) \pi / 2 \right]$ if $h/2 + ih < 1$, $\tilde{\phi}_i^0 = 1$ otherwise.

To obtain the stationary solution, we perform all the simulations until
$$\max_{i=0}^{n} \frac{\tilde{\phi}_i^{\,j+1} - \tilde{\phi}_i^{\,j}}{m} < 10^{-9}.$$

For all the cases, the maximum simulation time does not exceed 7.4.

The results of the computations are presented in Figs. 1 and 2 (case 1), 3 (case 2), 4 (case 3), 5 (case 4), 6 (case 5).

For the values of r not shown in the figures $\phi \approx 1$. The graphs of the solution were plotted as the computed values of $\tilde{\phi}_i^{\,j}$ are related to the cell centers, connected by straight line segments. In the vicinity of $r = 0$, we use a finer, sub-cell, visualization mesh to show the asymptotic behavior of the basis functions which were used during the computations.

Note that if the bi-Laplacian operator is present in the equation (i.e., $\alpha \neq 0$), the solution can be non-monotone and, at some points, achieve values grater than 1 (see Figs. 3 and 5). Such behavior was also noted in [3]; to avoid this, it was suggested to use relatively small values of α.

The numerical experiments confirm that the proposed finite-difference scheme is appropriate for accurate simulation of the problem solution, even in situations where the solution has singular behavior in the vicinity of $r = 0$.

5. Conclusion

The present work continues the study started in the article [3]. As noted by its authors, although the study is performed for a specific problem, it probably touches certain fundamental issues related to the application of the diffuse interface approach in general. The essence of these issues is whether diffuse interface models in their "classical" version allow one to adequately describe inclusions that are by their nature objects of higher co-dimension. As a possible answer, the authors of the paper [3] propose a generalization of the original model.

The aim of this work was to numerically investigate the above-mentioned generalization. Using a modification of the finite volume method, the difficulties associated with the need to specify boundary conditions on sets of co-dimension 2 and 3 in three-dimensional space and with the presence of a singularity in the solution at the points of these sets were overcome. The indicated approach is not
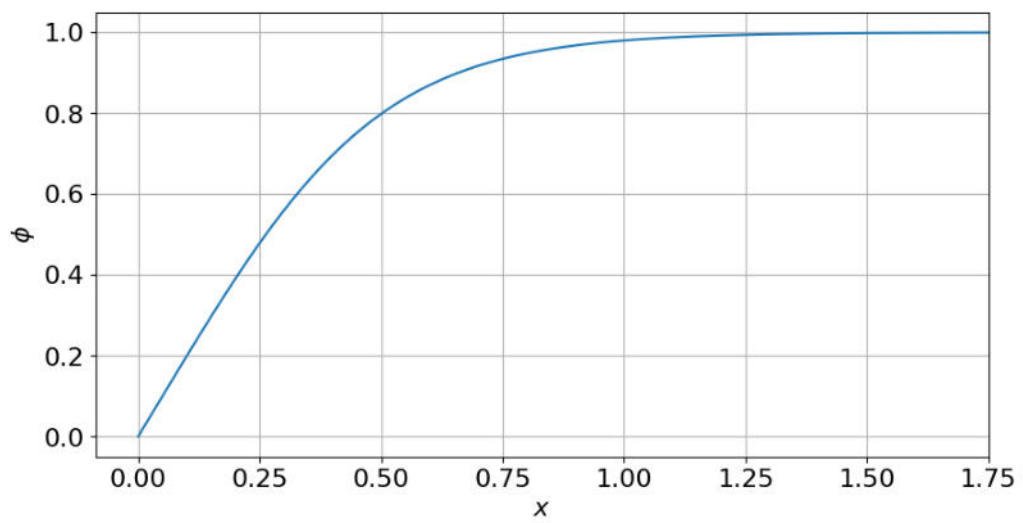
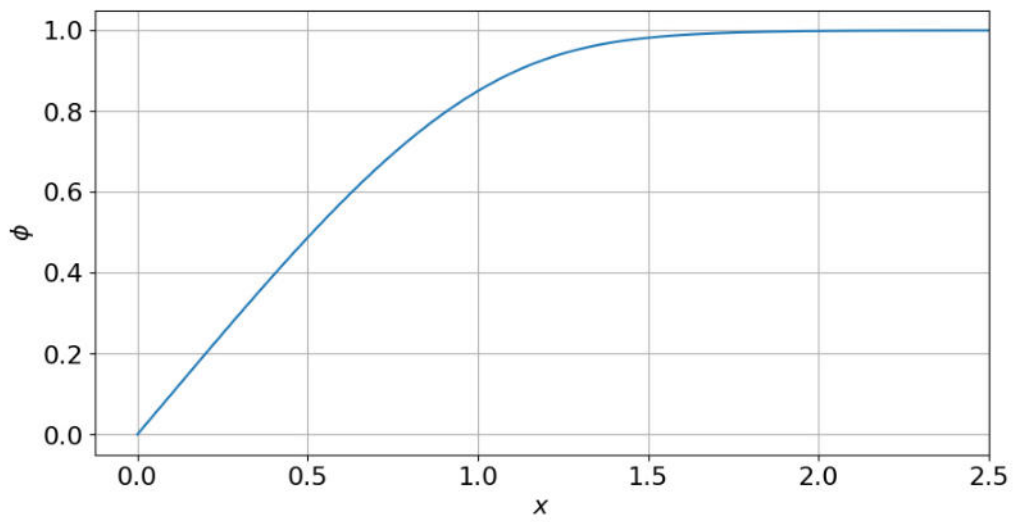Figure 1. The solution ϕ for the planar case with $\alpha = 0$, $\beta = 0$.

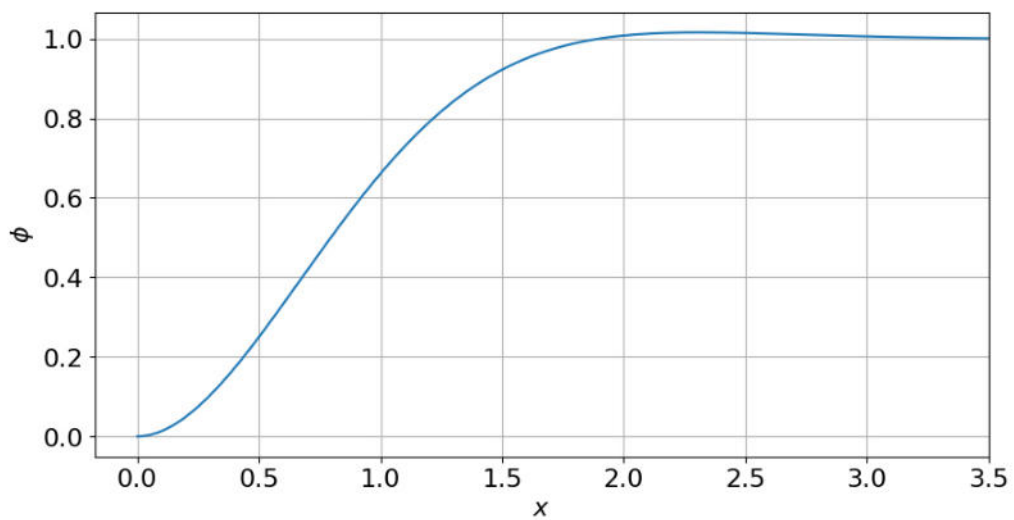Figure 2. The solution ϕ for the planar case with $\alpha = 0$, $\beta = 1$.

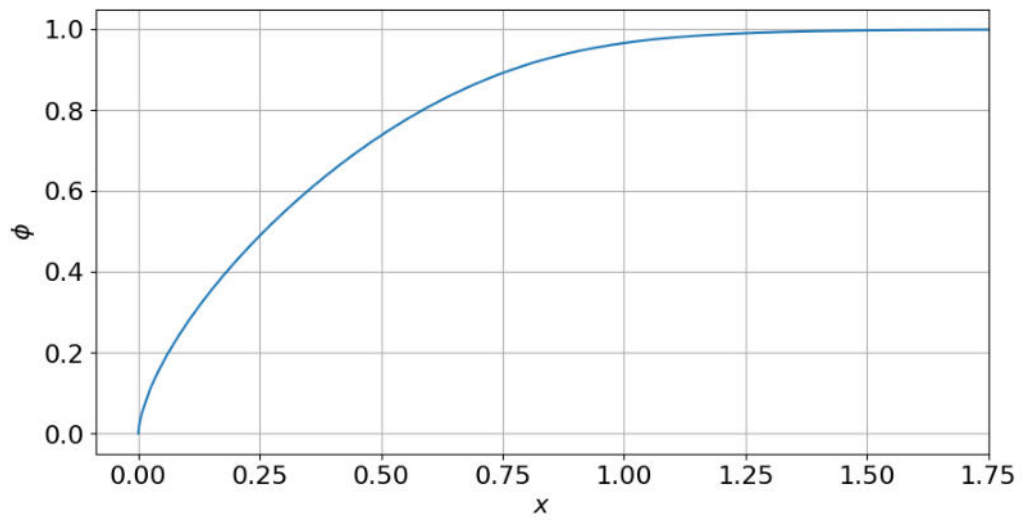Figure 3. The solution ϕ for the planar case with $\alpha = 1$, $\beta = 0$.

Figure 4. The solution ϕ for the axisymmetric case with $\alpha = 0$, $\beta = 1$.

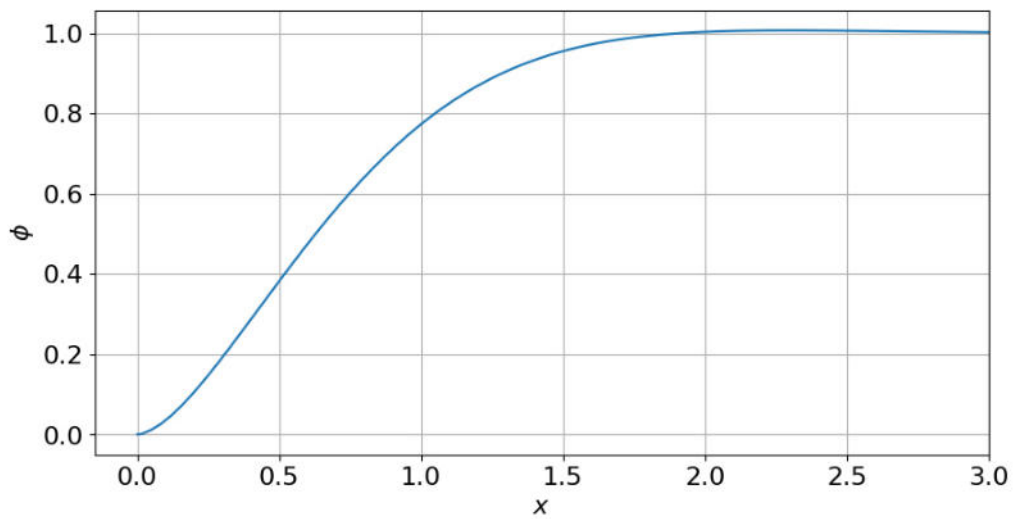Figure 5. The solution ϕ for the axisymmetric case with $\alpha = 1$, $\beta = 0$.
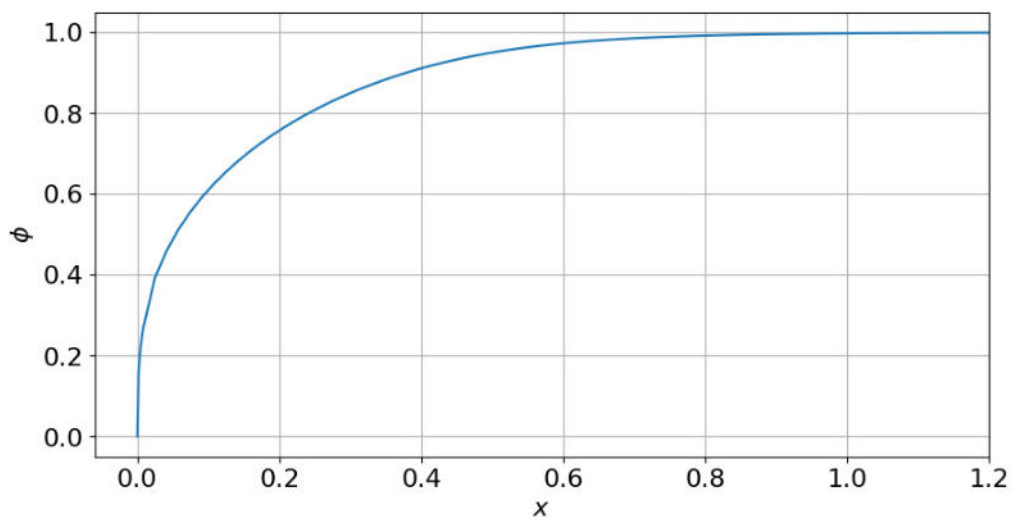

Figure 6. The solution ϕ for the spherically symmetric case with $\alpha = 0$, $\beta = 1$.

essentially tied to the model under consideration — in the future it can be used to analyze other problems.

In some of the cases considered, fundamental obstacles arose when constructing the finite-difference scheme: it turned out that the necessary basis functions simply did not exist. Based on this, a hypothesis was put forward that in these cases the differential problem under consideration is posed incorrectly and has no solution. This reasoning is in full agreement with the theoretical results of the work. In fact, while constructing the finite-difference scheme, the singular behavior of the solution was studied. Exactly the same approach can be used in order to study such singularities form a theoretical point of view, without any regard to construction of a numerical algorithm.

The presented reasoning is quite consistent with the theoretical results of the work [3]. In the future, a rigorous substantiation of the presented hypothesis is possible.

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