On the diffuse interface models for high codimension dispersed inclusions

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Abstract

Diffuse interface models are widely used to describe evolution of multi-phase systems of different nature. Dispersed “inclusions”, described by the phase field distribution, are usually three dimensional objects. When describing elastic fracture evolution, elements of the dispersed phase are effectively 2d objects. An example of the model which governs evolution of effectively 1d dispersed inclusions is phase field model for electric breakdown in solids. Phase field model is defined by appropriate free energy functional, which depends on phase field and its derivatives. In this work we show that codimension of the dispersed “inclusion” significantly restrict the functional dependency of system energy on the derivatives of the problem state variables. It is shown that free energy of any phase field model suitable to describe codimension 2 diffuse objects necessary depends on higher order derivatives of the phase field or need an additional smoothness of the solution — it should have first derivatives integrable with a power greater then two. To support theoretical discussion, some numerical experiments are presented.

Keywords: diffuse interface models; phase field; order parameter; electric breakdown

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I. INTRODUCTION

Phase-field (or order parameter) models constitute a powerful and theoretically sound framework for analysis of a broad class of theoretical and applied problems in multi-phase hydrodynamics [1–5], solid mechanics and fracture [6], material science [7], solidification and phase transitions [8–11], crystal structures [12–14] and many others topics.

The purpose of this class of models is, in general, a description of the dynamics of certain “inclusions” — elements of the dispersed phase immersed into homogeneous medium. Such inclusions are usually elementary macroscopic constituents (e.g., drops) of the dispersed phase of some multi-phase system. Spatial distribution of the dispersed phase is described by the so-called phase field or order parameter field which is a smooth function of time and spatial coordinate. Phase field function is almost constant inside spatial domain occupied by the phase and changes rapidly in the neighbourhood of the inter-phase boundaries. For example, in the context of multi-phase hydrodynamics, diffuse interface separates two immiscible fluids. Diffuse interface is always of the finite width (hence the term) which is a model parameter. Respectively, diffuse interface models have to provide internal mechanisms which prevent excising sharpening or spreading of the diffuse interface during system evolution. This makes the diffuse interface much more than just smoothed out contact discontinuity.

Comprehensive theoretical, applied and numerical analysis of the diffuse interface models is a topic of huge amount of literature. Either of these fields is a complex and complicated subject — in particularly because of necessary non-linearity of such models.

One of the central concepts of the diffuse interface models is the so-called “sharp interface limit” of the diffuse model. Roughly speaking, the sharp interface counterpart of the diffuse interface model is a model that is raised up when the diffuse interface width tends to zero. For example, sharp interface limiting model for multi-phase hydrodynamics is a free-boundary type model with sharp inter-phase boundaries considered as two-dimensional surfaces complemented by the respective interface conditions for conservative variables and their fluxes. Transition from the diffuse interface model to the respective sharp interface one usually is performed using asymptotic analysis and/or $\Gamma$-convergence framework [15–21].

The connection between diffuse interface model and its sharp interface counterpart is rather intimate. On the one side, for a number of diffuse interface models the existence of it’s physically meaningful sharp counterpart gives theoretical and practical ground to the former
one. On the other side, thermodynamically consistent procedures to derive constitutive relations for phase field models (using Coleman-Noll procedure or Liu framework) can be applied only if provided with expression of the energy of the system defined as a function of its primary thermodynamical variables and their gradients. This dependency can not be specified in more or less precise way from the thermodynamical considerations — rather it is the departure point of the consistent derivation — and has to be postulated somehow else. In many cases sharp interface limiting model (considered now as a primary one) is a source of suitable thermodynamic relations, see, e.g. [24].

The topic of this paper is to consider such feature of the diffuse interface models as spatial dimension (or codimension) of the “inclusion” which evolution is described by the phase field model.

For example, for diffuse interface models of multiphase hydrodynamics, such “inclusions” are just droplets of the dispersed phase. Both continuous (dispersion) phase and dispersive phase occupies effectively 3d spatial domains. In this case the inclusion have dimension 3 and, hence, codimension 0. The interphase boundary is effectively a 2d object with codimension 1. For diffuse models of fractures the “inclusion” represents fracture mid-surface which is effectively of the dimension 2 in 3d setting (and, respectively, of codimension 1).

Up to the authors knowledge, the only example of the phase-field model which governs evolution of the codimension 2 (i.e., 1d objects embedded in 3d medium) is presented in the work [25] which deals with phase field model for electric breakdown of the non-conducting dielectric medium.

The goal of the present paper is to show that codimension of the diffuse “inclusion” (or, more precisely, codimension of its sharp interface counterpart) significantly restrict the functional dependency of system’s energy on the derivatives of the problem state variables. In particular, keeping the form of this dependency as in the lower codimension case, when considering models with higher codimension “inclusion”, can lead to the mathematically incorrect problem setting.

Specifically, we show that a model suggested in [25] can not be used to describe electric breakdown channel as effectively one-dimensional object. At the same time, description of the breakdown channel as the three dimensional object doesn’t need constructions described in [25]. Based on certain formal considerations we propose corrected version of the phase field electric breakdown model.
The aforementioned model \cite{25} is considered as a specific example of the phase field model of “codimension two”. Nevertheless, we suppose that the presented considerations are of the general interest and importance.

II. PRELIMINARY DISCUSSION

The subject of this paper is the diffuse interface model for description of electric breakdown process in solid dielectric medium suggested in \cite{25,26} and further used in \cite{27,31}. The model \cite{25} is constructed as a formal generalization of the well known phase field models for fracture evolution in elastic medium. The derivation of the model is based on the formal analogy between breakdown channel evolution and evolution of the fracture in an elastic medium.

The motivation for such generalization is based on the following considerations.

In traditional theories of elastic fracture mechanics \cite{32,33}, the fracture mid-surface is described as a sufficiently smooth two-dimensional surface $\Gamma$ embedded into the three-dimensional space — i.e., as a geometrical object of codimension $\text{codim} \Gamma = 1$. Similarly, electric breakdown channel $\Lambda$ can be considered as a segment of one-dimensional curve embedded into the three-dimensional space — being a geometrical object of codimension $\text{codim} \Lambda = 2$.

In both cases, the evolution of codimension 1 fracture mid-surface or codimension 2 breakdown channel is governed by an appropriate internal forces, of the elastic or quasi(electro)static nature, acting in the medium. Besides this, for both fracture surface and breakdown channel, it is possible to construct the so called $J$-integral, which describes energy release rate during fracture or channel evolution.

For fractures the concept of $J$-integral is well known since fundamental works of G. Cherepanon \cite{32} and J. Rice \cite{34}. For breakdown channel evolution, $J$-integral was derived in \cite{35}. In this paper the breakdown channel is described as one-dimensional conducting curve which “growth” inside non-conducting medium. In both cases (for elastic fractures and breakdown channel), $J$-integral can be used to define fracture or channel growth criterion.

This formal correspondence between the processes (qualitatively, the only formal difference between them is their codimension) motivates authors of \cite{25} to extend formally phase field fracture models to phase field models for breakdown channel evolution.
To proceed, let us briefly discuss two main approaches for construction of phase field models for fractures, see, e.g. [6] for comprehensive review.

The first approach, which is referred to as “mechanistic” hereinafter, is based on the framework of the variational fracture theory, see [21], [20, Chapter 3] and references there. It is based on the following constructions.

Consider spatial domain \( \Omega \subset \mathbb{R}^n \) \( (n = 1, 2, 3) \), occupied by physically and geometrically linear homogeneous elastic medium, to which an external surface and volumetric forces are applied. Let \( \Gamma \subset \Omega \) be the fracture mid-surface. In the two-dimensional setting \( \Gamma \) is considered as segment of a smooth curve, in three-dimensional one — as a smooth surface with boundary. Within the variational fracture theory (hereinafter we follow [20, 21, 36]) the energy of the system has the form of

\[
J = J(u, \Gamma) = \int_{\Omega \setminus \Gamma} W(\nabla \otimes u) \, d\Omega + \kappa H^{n-1}(\Gamma),
\]

with \( u \) being the displacement field, \( H^{n-1}(\Gamma) \) — \((n-1)\)-dimensional Hausdorff measure, \( \kappa \) being the specific energy attributed to the unit surface element of the fracture mid-surface. The dimension of the Hausdorff measure is essential here: fixing it to be equal to \( n - 1 \), one explicitly states that fracture is the geometrical object of codimension 1.

The functional (1) is the departure point for development of the variational fracture theory. It can be shown that, under certain assumptions which are of no importance now, the displacements \( u \) of the medium and the trajectory \( \Gamma(t) \) of the fracture are minimizers of (1) at each moment of time. The details of the variational fracture theory are not presented further, they are widely described elsewhere.

In the specified setting the analysis of the problem is complex — both from the theoretical and numerical points of view: to solve the problem one need to be able to compute variations of (1) in respect to the fracture mid-surface configuration, that is, in respect to \( \Gamma \).

For this reason, it is more convenient to approximate the Hausdorff measure in (1) by the volume integral as (see [21, 36])

\[
H^{n-1}(\Gamma) \approx \int_{\Omega} \gamma_l(\phi, \nabla \phi) \, d\Omega,
\]

where volumetric approximation of the surface energy density reads

\[
\gamma_l(\phi, \nabla \phi) = \frac{1}{2l} \phi^2 + \frac{l}{2} \| \nabla \phi \|^2,
\]

(2)
In this case the energy functional (1) is approximated by

\[
\mathcal{J} \approx \mathcal{J}_l = \mathcal{J}_l(u, \phi, \nabla \phi) = \int_{\Omega} ((1 - \phi)^2 + \epsilon) W(\nabla \otimes u) \, d\Omega + \int_{\Omega} \kappa \gamma_l(\phi, \nabla \phi) \, d\Omega, \tag{3}
\]

where the order parameter (phase field) \( \phi \) takes the value \( \phi = 1 \) on the fracture mid-surface \( \Gamma \) and \( \phi = 0 \) in undamaged material.

In (3), \( 0 < \epsilon \ll 1 \) is a small real valued parameter which prevents degeneracy of the functional when \( \phi = 1 \). Usually it is chosen to be strictly positive — although it is known, that even with vanishing \( \epsilon \), the functional (3) is not degenerate, see \([37]\). It can be shown that (3) \( \Gamma \)-converges to the functional (1) when \( l \rightarrow 0 \).

If the fracture mid-surface \( \Gamma \) is prescribed and displacement field is vanishing (i.e., the median is not loaded), then it is easy to show that the distribution of \( \phi \) in space is defined as the minimizer of the functional

\[
\tilde{\mathcal{J}}_l = \tilde{\mathcal{J}}_l(\phi, \nabla \phi) = \int_{\Omega} \kappa \gamma_l(\phi, \nabla \phi) \, d\Omega, \tag{4}
\]

subjected to the boundary conditions

\[
\phi|_{\Gamma} = 1; \quad \phi \rightarrow 0, \ x \rightarrow \infty. \tag{5}
\]

The corresponding Euler-Lagrange equations read:

\[
-\Delta \phi + \frac{1}{l^2} \phi = 0, \quad x \in \Omega. \tag{6}
\]

It can be shown that in 1d case \( n = 1, \Gamma = \{x_0 = 0\} \), the solution of the latter equation is

\[
\phi(x) = \exp(-|x|/l)
\]

and decreases exponentially as the distance from a point in space to the fracture mid-surface increases. In the multidimensional case, this property also holds. Now it can be seen that parameter \( l \) in the expression for \( \gamma_l \) defines the width of the diffuse fracture.

The equation (6) above is the model one. In the complete formulation of the problem, when the path \( \Gamma(t) \) of the fracture evolution is not known a priori, this equation is solved in the whole domain \( \Omega \) with a source term which depends on the local elastic energy of the medium. The points in space at which the value \( \phi = 1 \) are assumed to be the points of
the fracture. As a result, a new fracture surface (that is, a set of points where $\phi$ takes the value 1) is formed where, for example, sufficiently large tensile elastic stresses appears.

The second approach, which will be further called “thermodynamic”, is based on a-priory definition of the form of energy functional. With this definition, one postulates or derives, within the rational thermomechanics framework, the equations defining the fracture evolution and the state of the surrounding medium. These equations have a standard form, typical for a phase-filed models — in particular, the evolution of the order parameter $\phi$ is usually described by a classical equation of the Allen-Kahn type.

Note that both approaches are closely related in the sense that using a mechanistic approach, thermodynamically consistent models can be derived. However, their correctness must be proved a-posteriory — in contrast to the thermodynamic models, which are correct by construction. Neither of two methods is “more correct” or “less correct”. Indeed, in thermodynamic models it is necessary to define, from the very beginning, the form of energy of a medium with a fracture — which cannot be predicted by purely phenomenological considerations. An understanding of how this energy can be defined comes from considering “mechanistic” models.

An issue which is not explicitly discussed in the literature — and which is the topic to which the present work is devoted, — is the following. The choice of an expression for the energy density $\gamma_l$ and the corresponding functional (2) is not unique and has a certain arbitrariness. Nevertheless, definitely, the energy has to be chosen in such a way, that a minimization problem statement for the functional

$$\tilde{J}_l = \int_{\Omega} \gamma_l \, d\Omega \rightarrow \min,$$

subjected to the boundary conditions (5) is mathematically correct.

In the case when the “diffuse” object is a part of the surface in three-dimensional space, — that is, its sharp counterpart has codimension 1 — such questions do not arise since the boundary value problem is usually posed in the domain which boundary has its natural codimension 1 (i.e., it is a two-dimensional surface in three-dimensional case or one-dimensional in two-dimensional case) — and in this sense it does not differ from the boundary $\partial \Omega$ of the domain $\Omega$, $\dim \Gamma = \dim \partial \Omega = 2$. Obviously, if a diffuse object has larger codimension, the issue described above should be taken into account.

Consider now the diffuse interface model of the breakdown channel, presented in [25].
Essentially, it is constructed as a formal generalization of the fracture diffuse model. In particular, it is implicitly assumed that the behavior of the system is described by the energy functional, which has the form (cf. (1))

\[ J = J(\Phi, \Gamma) = \int_{\Omega \setminus \Lambda} W(\nabla \otimes \Phi) \, d\Omega + \kappa \mathcal{H}^{n-2}(\Lambda), \]

where \( \Phi \) is electric field potential, \( \mathcal{H}^{n-2}(\Lambda) \) stands for \( n-2 \)-dimensional Hasudorff measure, \( \kappa \) is equal to the specific energy assigned to the unit length of the breakdown channel. The dimension of the Hausdorff measure is essential here: this time it is equal to 2 (in 3d case), which explicitly says that breakdown channel is a 1d object embedded in 3d space.

The key point now is the question of how should the corresponding part of the energy (that is, \( \gamma_l \)) of the system be specified in order to approximate in the correct way the values of

\[ \mathcal{H}^{n-2}(\Gamma) \approx \int_{\Omega} \gamma_l(\phi, \nabla \phi) \, d\Omega, \]

subjected to the boundary conditions (5). The answer to this question essentially depends on the codimension of \( \Lambda \). As it will be shown below, the expression (2) cannot be used if \( \Lambda \) has codimension 2, i.e., if \( \Lambda \) is a curve in 3d case or a point in planar case.

Note that the expressions (7) and (8) with the boundary conditions (5) essentially defines the capacity of the set \( \Lambda \) relative to \( \gamma_l \). Therefore, the question of the correctness of the considered minimization problems is closely related to the theory of the capacity of sets — in particular, with the question of whether the capacity of a set of a given codimension is positive — informally, that is the criteria to check if the set \( \Lambda \) supports definition of the boundary condition of the given type.

### III. FORMAL DESCRIPTION OF THE MODEL FROM [25]

Let us briefly outline the phase field model proposed in [25] to describe electric breakdown channel propagation in a solid dielectric.

Consider a bounded domain \( \Omega \) occupied at the initial time \( t = 0 \) with a solid dielectric with electric permeability \( \epsilon = \epsilon_0(x, t) \). During the electrical breakdown, the formation of a breakdown channel occurs. The physical breakdown channel can be described as a cylindrical domain of small radius. By analogy with fractures in an elastic medium, this domain
is considered as a damaged domain with alternative properties. According to the diffuse interface method, it is assumed that the spatial distribution of the damaged material is described by at least continuous scalar function (phase field or order parameter) \( \phi = \phi(x, t) \), defined in \( \Omega \). The range of this function is a segment \([0, 1]\), its value \( \phi = 0 \) corresponds to the medium in the breakdown channel, the value \( \phi = 1 \) — to the undamaged medium. The values \( \phi \in (\epsilon, 1 - \epsilon) \), \( \epsilon \ll 1 \) correspond to the diffuse boundary separating the breakdown channel \( (\phi = 0) \) from the intact medium \( (\phi = 1) \). Equations defining the evolution of the order parameter \( \phi \) are chosen so that the channel domain is a small tubular neighborhood of a curve in space that corresponds to the axis (middle curve) of the breakdown channel. The effective diameter of this tubular neighborhood in equilibrium state is defined by a model parameter.

Assuming the breakdown channel be an ideal conductor, its electric permittivity is infinitely large. In the model, in accordance with the ideas of the diffuse interface approach, the permittivity is assumed to have finite, but very large values. Specifically, it is defined as

\[
\epsilon = \epsilon[\phi](x, t) = \frac{\epsilon_0(x)}{f(\phi(x, t))} + \delta. \tag{9}
\]

Here \( \epsilon_0 = \epsilon_0(x) \) is electric permittivity of the undamaged medium; \( f = f(\phi) \) is the so called interpolation (or degradation) function; \( 0 < \delta \ll 1 \) is a small positive real valued regularizing parameter, which prevents degeneracy of \( \text{(9)} \) at \( \phi = 0 \).

The main role of the function \( f \) is the interpolation of the medium properties and parameters of the model between the damaged and undamaged values, which corresponds to the "pure" phases identified by \( \phi = 0 \) and \( \phi = 1 \), see [38]. In [25], it is chosen as \( f(\phi) = 4\phi^3 - 3\phi^4 \).

Since the development of the breakdown channel is essentially slower than the speed of electromagnetic waves propagation in the medium, it is assumed that the energy of the magnetic field can be neglected. As a result, the problem is considered in quasi (electro)static setting and distribution of the electric field is potential.

As a result, within the formal analogy with phase field fracture models, the following dependency of free energy on state variables and their derivatives is postulated in [25]:

\[
\Pi = \int_{\Omega} \pi d\Omega, \quad \pi = \pi(\Phi, \phi, \nabla \phi), \tag{10}
\]
\[ \pi = -\frac{1}{2} \mathbf{E} \cdot \mathbf{D} + \Gamma \frac{1 - f(\phi)}{l^2} + \frac{\Gamma}{4} \nabla \phi \cdot \nabla \phi = \]
\[ = -\frac{1}{2} \epsilon(\phi) \nabla \Phi \cdot \nabla \Phi + \Gamma \frac{1 - f(\phi)}{l^2} + \frac{\Gamma}{4} \nabla \phi \cdot \nabla \phi. \]  
(11)

with \( \mathbf{E} = -\nabla \Phi \) being the electric field, \( \Phi \) being its potential, \( \mathbf{D} = \epsilon \mathbf{E} \) being the electric induction; \( \Gamma \) is specific energy per unit length of the channel and \( l \) defines its effective radius.

The first term in (11) is the electrostatic energy of the medium. Other terms are “phase field part” of the energy and are chosen by the authors of [25] formally — they coincide with that for the energy used in the diffuse fracture models. The primary state parameters of the model are \( \Phi, \phi \) and \( \nabla \phi \).

The system of equations that describes evolution of the system in the non-stationary case is postulated in the form

\[ \frac{\delta \pi}{\delta \Phi} = 0, \]
(12a)

\[ \frac{1}{m} \frac{\partial \phi}{\partial t} = -\frac{\delta \pi}{\delta \phi}. \]
(12b)

Above, the first equation (12a) describes the distribution of electric potential \( \Phi \). The second one is the simplest equation describing the kinetics of the order parameter. The parameter \( m > 0 \) is phenomenological parameter called mobility with the meaning of the rate of change of a given quantity under the action of a applied unit force. The equation (12b) formalizes the empirical assumption that the deviation of the spatial distribution of the order parameter from the equilibrium state evolves so that to compensate the deviation.

In the expanded form equations (12) read:

\[ \nabla \cdot (\epsilon(\phi) \nabla \Phi) = 0, \]
(13)

\[ \frac{1}{m} \frac{\partial \phi}{\partial t} = \frac{1}{2} \epsilon'(\phi) \nabla \Phi \cdot \nabla \Phi + \Gamma \frac{f'(\phi)}{l} + \frac{\Gamma}{2} \Delta \phi, \]
(14)

where \((\cdot)' \equiv (\cdot)'_{\phi}\) and dependency \( \epsilon = \epsilon(\phi) \) is defined by (9).

The first equation above is the equation for the electric potential with a dielectric permittivity depending on the distribution of the order parameter. The second equation has the form of an Allen-Cahn type equation which describes the spatial and temporal evolution of the order parameter.

The equilibrium state of the medium with free energy defined by (11) is defined by the conditions of vanishing variations of (11) in \( \Phi \) and \( \phi \). The corresponding Euler-Lagrange
equations are formally correspond to the equations (12) with $1/m \to 0$ and have the form of:

\[
\nabla \cdot (\epsilon [\phi] \nabla \Phi) = 0, \quad \frac{1}{2} \epsilon' [\phi] \nabla \Phi \cdot \nabla \Phi + \frac{\Gamma}{l^2} f'(\phi) + \frac{\Gamma}{2} \Delta \phi = 0. \tag{15}
\]

To determine the structure of the diffuse interface described by the model (15), consider an unbounded domain in which the axis of the breakdown channel is a smooth curve $\Lambda$. Assuming the vanishing electric field in the medium, the order parameter $\phi$ satisfies the following boundary conditions:

for $x \in \Lambda$ : $\phi(x) = 0$,

for $x \to \infty$ : $\phi(x) \to 1$,

and the governing equation:

\[
\frac{\Gamma}{l^2} f'(\phi) + \frac{\Gamma}{2} \Delta \phi = 0 \tag{16}
\]

defined in $\mathbb{R}^3 \setminus \Lambda$.

The solution to this equation describes the distribution of the order parameter, which corresponds to the straight conductor of infinitely small diameter. Here, a conductor is understood as a set of points in space with $\epsilon = +\infty$, which corresponds to the value $\phi = 0$.

Define cylindrical coordinate system $O r \theta z$, with $r$ being the distance from a point in space to the axis $O z$ and $\theta$ being the polar angle. In what follows, we will assume that the breakdown channel coincides with the $O z$ axis, that is, $\Lambda = O z$ and the order parameter distribution $\phi$ depends only on the radius, i.e., $\partial \phi / \partial \theta = \partial \phi / \partial z = 0$ and $\phi = \phi(r)$.

In [25] it is stated that axisymmetric distribution of the order parameter satisfy the equation

\[
f'(\phi) + \frac{r^2 d^2 \phi}{2 dr^2} = 0 \tag{17}
\]

with boundary conditions

$\phi |_{r=0} = 0$; $\phi |_{r\to\infty} \to 1$. \tag{18}

Integration of (17) leads to the equation

\[
\frac{d \phi}{d r} = \frac{2}{l} \sqrt{1 - f(\phi)}. \tag{19}
\]

In [25], equations (17) and (19) are equations (13) and (14).
The model described in the previous section is the only model known to the authors in which the diffuse interface model is used to describe an object with codimension 2. Although the method of its construction is the “mechanistic” one, it is relatively common and widely used.

Nevertheless, its particular implementation in [25] is not completely correct. More precisely, the form of free energy used to describe a (codimension 1) “diffuse” fracture cannot be used to describe a (codimension 2) “diffuse” breakdown channel. As will be shown below, this is due to the fundamental mathematical properties of the corresponding expression for the free energy.

First, the equation (17), which is positioned [25] as an equation describing an axisymmetric distribution of the order parameter, is incorrect.

Indeed, consider the primary equation (16) for the phase field distribution in the three-dimensional domain, which contains an infinitely long breakdown channel.

Let us remind definition of the Laplace operator in the cylindrical coordinates $\mathcal{O}r\theta z$,

\[
\Delta \phi = \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \phi}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 \phi}{\partial \theta^2} + \frac{\partial^2 \phi}{\partial z^2}. \tag{20}
\]

For one dimensional axially symmetric case ($\partial \phi/\partial z = \partial \phi/\partial \theta = 0$), considered in [25], it followos from (16) and (20) that

\[
\frac{1}{l^2} f'(\phi) + \frac{1}{2} \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \phi}{\partial r} \right) = 0, \tag{21}
\]

or, expanding derivatives,

\[
\frac{1}{l^2} f'(\phi) + \frac{1}{2} \left( \frac{1}{r} \frac{\partial \phi}{\partial r} + \frac{\partial^2 \phi}{\partial r^2} \right) = 0. \tag{22}
\]

First of all let us note that equations (21) and (22) differs form (17) and (19), given in [25] as equations (13) and (14). It is easy to notice that (17) and (19) are correct, but only for one dimensional planar case and not for the axysimmetric one as it is stated in [25].

This error would be rather technical one if not for the following observation.

To construct a solution to the one-dimensional equation (22), the boundary conditions (18) with respect to solution values has to be accounted at point $r = 0$ and $r \to +\infty$. 

IV. ANALYSIS OF THE MODEL [25]
It is well known that setting the boundary condition at \( r = 0 \) (which is a point set) on the value of the solution to determine axisymmetric solutions of the second order equation of the type (16) is incorrect. The rationale for this statement is the presence of the so-called theorems on “removable isolated singularities” in the theory of PDEs. In particular, such a result is well known in the theory of harmonic functions. Simply speaking it states that if a function is bounded and harmonic outside any arbitrarily small neighborhood of the given point, then it can be extended to this point as harmonic function. This means that the value of such function can not be defined arbitrarily at a single point.

The equation (16) considered here is not the Laplace equation, but is the second order semi-linear elliptic equation with Laplacian as a leading term. Consider it in the two-dimensional case (that is, \( \partial \phi / \partial z = 0 \)). The requirement for the axisymmetry of the solution is no longer will be needed. For (16) the required result is given in [39, 40] and can formulated as follows (see also [41, 42]):

Consider equation (16) defined in the domain \( \Omega \subset \mathbb{R}^2 \). Let \( \phi = \phi(x) \) be its solution in \( \Omega \setminus \omega(x_0) \) with \( \omega(x_0) \) being an arbitrarily small neighborhood of the point \( x_0 \in \Omega \). Then \( x_0 \) is removable singularity — that is, \( \phi = \phi(x) \) can be extended to \( \Omega \) as the solution of (16) iff \( \phi \) growth not faster than \( \mu(x) = \ln(1/\|x - x_0\|) \), i.e., \( \lim_{x \to x_0} \phi(x)/\mu(x) = 0 \).

The boundary condition \( \phi(x_0) = \phi_0 \) with finite \( \phi_0 \) at the point \( x_0 = 0 \) ensures fulfillment of these conditions. Hence, \( \phi(x) \) satisfies equation (16) in whole domain \( \Omega \) with boundary conditions defined at its outer boundary. For axisymmetric problem with \( \Omega \) being a disk of the given radius centered at \( x_0 = 0 \) and boundary conditions (18) at \( r = R \) or \( r \to +\infty \), such solution is the trivial one, i.e., \( \phi(x) = 1 \).

From here it follows that overall setting considered in [25] is not mathematically correct — since point boundary conditions can not be set for semilinear 2-nd order PDEs of the considered form.

Thus, the results presented in [25], in particular, equation (13), (14) and the solution in figure 2 (here the references are given according to [25]) are not correct — they describe the planar case, which corresponds to the diffuse interface models for fractures and is mathematically sound.

In this case, actually covered in [25], posing boundary conditions for the values of solution at \( r = 0 \) is possible — in the planar case the set of points \( r = 0 \) is a line on a plane (in a two-dimensional case) or a plane in space (in 3d setting). In other words, the equation (16)
in this case is considered in the half-space $0 < x_1 < +\infty$, where $x_1 \equiv r$.

Note that the equation (21) can be formally approximated by a suitable difference scheme in the domain $r \in [0, R]$ with a given Dirichlet boundary conditions at $r = 0, R$. In this case, the numerical solution will have a qualitative form, presented in figure 2 in [25]. However, when refining the mesh step size, there will be observed complete absence of grid convergence: with mesh step size going to zero, the solution will asymptotically tends to 1 at each point except for $r = 0$. In other words, the derivative of the numerical solution at the point $r = 0$ will be tend to zero at the point $r = R$ and to infinity at $r = 0$, see figure 1. However, as can be easily shown, this is not the case for the solution of the equation (19). Indeed, for $r \to 0$ we have $\phi \to 0$ and from the equation (19) it follows that $d\phi/dr \to 1$. Similarly, if the equation (19) is solved in the region $0 < r < R < +\infty$ with the boundary condition $\phi(r = R) = 1$, then for $r \to R$ we have $\phi \to 1$ and, as a consequence, $d\phi/dr \to 0$.

It can be assumed that the lack of numerical convergence was not discovered by the authors of [25] due to the fact that authors solve numerically not the “primary” equation (21) or (22), but the equation (19), which corresponds to the planar, not axisymmetric case.
Thus, the setting of the boundary conditions for equations (16) is not mathematically possible on the codimension 2 set Λ, which models the breakdown channel. To correct the model one need to modify expression (11) for the energy of the system in such a way, that for the corresponding Euler-Lagrange equation (16), definition of the Dirichlet boundary condition on Λ with codim Λ = 2 would be possible.

The easiest way to see how this can be done is to consider the equation (16) in weak (variational) setting. Consider the equation (16) in the two-dimensional domain Ω, which is assumed to be simply connected and without “punctured” points. In this case, the weak statement of the problem (16) in the two-dimensional region Ω ⊂ R^2 has the form: find a function u ∈ V such that

\[ a(u, v) + (f'(u), v) = 0, \quad a(u, v) = \int_\Omega \nabla u \cdot \nabla v \, d\Omega, \quad (f(u), v) = \int_\Omega f(u) v \, d\Omega, \]

for an arbitrary test function v ∈ V_0. Here the functional space V_0 ⊂ V consist of functions from V vanishing on ∂Ω, V is a space of sufficiently smooth functions defined in Ω. Here “sufficiently smooth” means that function from V have finite energy norm induced by the bilinear form a(·, ·).

For the second order elliptic problem (23) the natural smoothness is V = W^1_2(Ω), that is, the Sobolev space of functions which are L^2-integrable and have L^2-integrable gradient. Accordingly, the space V_0 = W^1_{2,0}(Ω).

Due to the well-known trace theorems (see [43, 44]), for functions v ∈ H^1(Ω) the trace operator is defined only for the sufficiently smooth manifolds of codimension 1, i.e., surfaces in 3d. For manifolds of codimension 2 — which is of the interest here — the trace of functions v ∈ H^1(Ω) cannot be defined. From here it is clear that boundary conditions can not be defined for a function from H^1(Ω) except the boundary is a codimension 1 manifold.

Consider Sobolev space W^q_p(Ω), Ω ⊂ R^n, n = 3, which can be defined as

\[ \|u\|_{W^q_p(\Omega)}^p = \sum_{|\alpha| \leq q} \|D^\alpha u\|_p^p, \quad \|\cdot\| = \|\cdot\|_{L_p(\Omega)}, \]

where α = (α_1, α_2, ..., α_n) is multi-index

\[ D^\alpha = \frac{\partial^{|\alpha|}}{\partial x_1^{\alpha_1} x_2^{\alpha_2} \cdots x_n^{\alpha_n}}, \quad |\alpha| = \alpha_1 + \alpha_2 + \cdots + \alpha_n. \]
According to the embedding theorems, one have
\[ W^q_p(\Omega) \subset C^{r,\alpha}(\Omega), \quad |\alpha| \leq q, \]
if
\[ n < pq, \quad \frac{1}{p} - \frac{q}{n} = -\frac{r + \alpha}{n}, \]
where \( C^{r,\alpha}(\Omega) \) is the respective Hölder space.

This means that functions for which the value of \( pq \) is sufficiently large, will be at least continuous. In the considered case, one have \( n = 3 \), so that
\[ pq > 3, \quad \frac{1}{p} - \frac{q}{3} = -\frac{r + \alpha}{n}. \]

Restricting ourselves to the minimal natural values \( p \) and \( q \) satisfying the last inequality, we have \( pq = 4 \), whence:
\[ p = 2, \quad q = 2 : \quad r = 0, \alpha = 1/2, \]
\[ p = 4, \quad q = 1 : \quad r = 0, \alpha = 1/4. \]

This means, that the traces of the order parameter \( \phi \) will be correctly defined on manifolds of codimension 2 if from the finiteness of the values of the functional \( \pi \) it will follow that \( \phi \in W^q_p(\Omega) \) with \( p \) and \( q \) given above — that is for \( \phi \in W^q_2(\Omega) \) for \( q \geq 2 \) and/or \( \phi \in W^1_p(\Omega) \) for \( p \geq 4 \).

In the first case the energy has to include at least the term
\[ \pi_{2,2} = \int_\Omega (\Delta \phi)^2 \, d\Omega. \]
Hence, the corresponding Euler-Lagrange equation will have the polyharmonic term of the form \( \Delta^2 \phi \). In the second case, the energy has to include at least the term
\[ \pi_{1,4} = \int_\Omega \frac{1}{p} \| \nabla \phi \|^p \, d\Omega, \quad p \geq 4. \]
Hence, the corresponding Euler-Lagrange equation will have the so called \( p \)-Laplacian term \( \Delta_p \phi \equiv \nabla \cdot (\| \nabla \phi \|^{p-2} \nabla \phi) \). In what further we consider only the case of \( p = 4 \).

Note that the boundary value problems for the polyharmonic equation \( \Delta^k u = f, \quad k = 2, 3, \ldots \), with boundary conditions defined at
\[ \Gamma = \Gamma_0 \cup \Gamma_1 \cup \Gamma_2 \cup \ldots, \]
with $\Gamma_k$ being a manifold of codimension $k$, $\dim \Gamma_k = k$, codim $\Gamma_k = n - k$, $n = \dim \Omega$, $\Gamma_0 \equiv \partial \Omega$, are studied in \cite{43, 45-47}.

Correctness of the boundary value problems for the quasilinear elliptic equation with $p$-Laplacian is considered in \cite{48}.

Note that the main results of the theory of boundary value problems with boundary conditions, given on manifolds of high codimension, was basically obtained in the context of the theory of capacity of sets. Namely, one can often assume that a manifold of high codimension supports definition of the boundary conditions if the corresponding manifold has positive capacity with respect to problem’s operator. Currently, the theory of (degenerate) partial differential equations in domains whose boundaries include sets of high codimension, is a new and actively developed topic of the ODE theory, capacity theory and geometric measure theory, see, e.g. \cite{49} and references therein.

Thus, if the kinetic equation (12b) describing the dynamics of the order parameter will include a polyharmonic operator and/or $p$-Laplacian term, then for its solution the setting of boundary conditions on a manifold of codimension 1 will make sense. This is the hint to correct the model from \cite{25}.

The formal generalization of the energy which ensures the correctness of the diffuse interface model of the breakdown channel has the form:

$$
\Pi = \int_\Omega \pi d\Omega, 
$$

$$
\pi = \pi(\Phi, \phi, \nabla \phi, \Delta \phi) 
= -\frac{1}{2} \epsilon'[\phi] \nabla \Phi \cdot \nabla \Phi + \frac{\Gamma_1 - f(\phi)}{l^2} + \frac{\Gamma_2}{4} \nabla \phi \cdot \nabla \phi + \alpha \frac{\Gamma^2}{8} (\Delta \phi)^2 + \beta \frac{1}{p} \Gamma^{p-2} \|\nabla \phi\|^p, 
$$

where $p \geq 4$ is even natural number, $\|\cdot\|$ is the standard Euclidean norm in $\mathbb{R}^3$, $\alpha, \beta \geq 0$ are positive real parameters, unequal to zero simultaneously, i.e., $\alpha + \beta > 0$.

The complete system of equations describing evolution of the electric potential $\Phi$ and order parameter $\phi$, has the form (12) or, in the particular case under consideration,

$$
\nabla \cdot (\epsilon(\phi) \nabla \Phi) = 0, 
$$

$$
\frac{1}{m} \frac{\partial \phi}{\partial t} = \frac{1}{2} \epsilon'(\phi) \nabla \Phi \cdot \nabla \Phi + \frac{f'(\phi)}{l^2} + \frac{\Gamma_2}{4} \Delta \phi - \alpha \frac{\Gamma^2}{4} \Delta^2 \phi + \beta \Gamma^{p-2} \nabla \cdot (\|\nabla \phi\|^{p-2} \nabla \phi). 
$$

A priori, one cannot state which one of the regularizing terms in the expression (24) and (25) is preferable either form thermodynamic or numerical point of views — or both are
needed. We only note that $\alpha > 0$ and $\beta = 0$ leads to the linear biharmonic term in (25b) which poses certain problems in numerical approximations. As will be shown below, this makes solution of (25b) to be smooth at points of $\Lambda$. The case $\alpha = 0$, $\beta > 0$ leads to $p$-Laplacian term in (25b) which is nonlinear, but of the second order.

A consequence of the second equation of (25) is the following model equation describing the evolution of the order parameter:

$$\frac{1}{m} \frac{\partial \phi}{\partial t} + \alpha \frac{\Gamma l^2}{4} \Delta^2 \phi - \beta \Gamma l^{p-2} \nabla \cdot (\|\nabla \phi\|^{p-2} \nabla \phi) - \frac{\Gamma}{2} \Delta \phi - \frac{\Gamma}{2} f'(\phi) = 0. \tag{26}$$

For $\beta = 0$ this equation is widely known as Swift-Hohenberg equation. It is the basic equation in phase-field crystal models. These models are under active development, starting from the fundamental work [50], see review in [12, 14]. Note that the original model proposed in [50] contains only a biharmonic term. Examples of Swift-Hohenberg type models which have both the biharmonic and the $p$-Laplacian terms are given in [52], see also references therein.

Note that derivation of the Swift-Hohenberg equations known in the literature is physically justified, and is not mechanistic in the sense of section I: the term, proportional to $\Delta^2 \phi$ in the expression for the energy for these models appears from physical considerations related to the form of the free energy function of the corresponding atomic system, see, e.g., [12, 51].

Finally, let us note that:

- An example of a high-order diffuse boundary model for fractures is given in [36]. The motivation for using such a model in the specified work is to improve the smoothness properties of of the solution and, as a consequence, the computational properties of the isogeometric finite element method used for numerical solution of the problem. Thus, the generalizations made in [36] are intended to be rather technical and is not related to the correctness of the diffuse interface model.

- As noted in [36], for diffuse boundary models of higher order (with biharmonic term) for fractures in an elastic medium, rigorous and complete results concerning $\Gamma$-limit of these models are not known. In other words, unlike for the classic diffuse interface models for fractures, it is not proven for high-order models, that they approximate the classic Griffiths model of fracture. Nevertheless, the results of numerical calculations suggest that this issue is rather technical.
VI. NUMERICAL EXPERIMENTS

The system of equations \(25\) is nonlinear and of the high order. So it is difficult to predict its properties, especially analytically. To get insight in its properties we provide below number of numerical experiments.

Consider equation \(26\) in the stationary case:

\[
\alpha \Gamma l^2 \Delta^2 \phi - \beta \Gamma p^{-2} \nabla \cdot \left( \| \nabla \phi \|^{p-2} \nabla \phi \right) - \frac{\Gamma}{2} \Delta \phi - \frac{\Gamma}{l^2} f'(\phi) = 0.
\]  \(27\)

Let \(x_i = L \tilde{x}_i, i = 1, 3\) with \(L\) being the characteristic length, \(\tilde{x}_i\) is dimensionless coordinates.

The dimensionless form of this equation is:

\[
\alpha \frac{(l/L)^4}{4} \tilde{\Delta}^2 \phi - \beta (l/L)^p \tilde{\nabla} \cdot \left( \| \tilde{\nabla} \phi \|^{p-2} \tilde{\nabla} \phi \right) - \frac{(l/L)^2}{2} \tilde{\Delta} \phi - f'(\phi) = 0,
\]  \(28\)

where \(\tilde{\nabla}\) and \(\tilde{\Delta}\) are Hamilton and Laplace operators in dimensionless coordinates.

If characteristic length is chosen as \(L = l\), one obtains:

\[
\frac{1}{4} \Delta^2 \phi - \beta \nabla \cdot \left( \| \nabla \phi \|^{p-2} \nabla \phi \right) - \frac{1}{2} \Delta \phi - f'(\phi) = 0.
\]  \(29\)

In what further only dimensionless equations will be considered with the tilde symbol omitted.

In this section we will study dependence of numerical solutions of equation \(29\) parameters values. The following properties if solution of the equation \(29\) are of the interest

- the solution range must be a segment \(\phi \subset [0, 1]\);
- distribution of phase-field must be monotonic;
- numerical convergence must be observed with reasonable refinement of the computational grid;
- phase-field function values closed to zero has to be concentrated in the sufficiently small neighbourhood of \(r = 0\), so that the solution goes to the asymptotic \(\phi \to 1\), \(\partial \phi / \partial r \to 0\) when \(r \to +\infty\) pretty fast.

One must notice that these properties are not obvious for the solution of considered equation.

Numerical simulations were performed for the one dimensional axisymmetric problem. We assume that:
• breakdown channel is aligned along axis \( O \z \) of cylindrical coordinate system \( O r \theta z \);

• solution of the equation \((29)\) doesn’t depend on \( z \)-coordinate and is axisymmetric, so \( \partial \phi / \partial z = 0 \) and \( \partial \phi / \partial \theta = 0 \).

In this case, solution of equation \((29)\) depends only on coordinate \( r \) defined in cylindrical domain

\[ \Omega = \{ z \in \mathbb{R}, \theta \in (0, 2\pi], r \in (0, R) \} \]

In the considered axisymmetric case the equation \((29)\) reads:

\[
\frac{\alpha}{4} \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial}{\partial r} \left[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \phi}{\partial r} \right) \right] \right) - \frac{\beta}{2} \frac{1}{r} \frac{\partial}{\partial r} \left( r \left[ \frac{\partial \phi}{\partial r} \right]^{p-2} \frac{\partial \phi}{\partial r} \right) - \frac{11}{2} \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \phi}{\partial r} \right) - f'(\phi) = 0. \tag{30}
\]

The boundary conditions are

for \( r = 0 \) : \( \phi(x) = 0, \frac{\partial \phi}{\partial r} \bigg|_{r=0} = 0 \),

for \( r = R \) : \( \phi(x) = 1, \frac{\partial \phi}{\partial r} \bigg|_{r=R} = 0 \),

when \( \alpha \neq 0 \) and

for \( r = 0 \) : \( \phi(x) = 0 \),

for \( r = R \) : \( \phi(x) = 1 \),

when \( \alpha = 0 \).

For numerical solution of the problem, a finite difference method was used.

Consider a non-uniform computational mesh with \( N \) nodes defined in \( \Omega = [0, R] \):

\[ 0 = r_0 < r_1 < \ldots < r_{N-2} < r_{N-1} = R. \]

Let \( \omega_{i+1/2} = [r_i, r_{i+1}] \) be mesh cells with centers denoted by \( r_{i+1/2} \),

\[ r_{i+1/2} = (r_i + r_{i+1})/2, \quad i = 0, N - 2. \]

The cell centers form a dual mesh with cells \( \omega_i = [r_{i-1/2}, r_{i+1/2}], i = 1, N - 1 \). In what further let \( \Delta r_{i+1/2} = |\omega_{i+1/2}| = r_{i+1} - r_i, i = 0, N - 2 \) be a mesh step size for the primary mesh, \( \Delta r_i = |\omega_i| = r_{i+1/2} - r_{i-1/2}, i = 0, N - 2 \) be a mesh step size for the dual mesh.

The values of \( \phi \) related to the nodes of primary and dual meshes are denoted as \( \phi_i \) and \( \phi_{i+1/2} \), respectively. The corresponding mesh function is denoted as \( \phi_h = (\phi_0, \phi_1, \ldots, \phi_{N-1}) \).
At the nodes of the primary mesh, the finite-difference approximation of the equation (30) is defined at the nodes of the primary mesh and read:

\[
\alpha \frac{1}{4} \Delta^2_h \phi_h - \beta \Delta_{p,h} \phi_h - \Delta_h \phi_h - f'_i = 0,
\]

with the discrete Laplace operator \( \Delta^2_h \phi_h \) defined as

\[
[\Delta^2_h \phi_h]_i = \frac{1}{r_i} \frac{1}{\Delta r_i} \left[ \frac{\phi_{i+1} - \phi_i}{\Delta r_{i+1/2}} - \frac{\phi_i - \phi_{i-1}}{\Delta r_{i-1/2}} \right], \quad i = 1, N-2.
\]

discrete \( p \)-Laplacian defined as:

\[
[\Delta_{p,h} \phi_h]_i = \frac{1}{r_i} \frac{1}{\Delta r_i} \left[ \phi_{i+1} - \phi_i \right]^{p-2} \left( \frac{\phi_{i+1} - \phi_i}{\Delta r_{i+1/2}} \right) - \frac{\phi_i - \phi_{i-1}}{\Delta r_{i-1/2}} \right] r_{i-1/2} \left[ \frac{\phi_i - \phi_{i-1}}{\Delta r_{i-1/2}} \right]^{p-2} \left( \frac{\phi_i - \phi_{i-1}}{\Delta r_{i-1/2}} \right) , \quad i = 1, N-2,
\]

and the discrete biharmonic operator \( \Delta^4_h \phi_h \) defined as:

\[
[\Delta^4_h \phi_h]_i = [\Delta_h \circ \Delta_h \phi_h]_i , \quad i = 2, N-3.
\]

In the expression above the term \( f'_i \) is defined as

\[
f'_i = f'(\phi_i).
\]

Let’s denote finite-difference approximation of spatial derivatives by the index \( h \), e.g., \( \partial_h \phi_h / \partial_h r \) is approximation to the \( \partial \phi / \partial r \).

For \( \alpha \neq 0 \) the difference equation (31) is defined at the nodes \( i = 2, N-3 \), i.e., in all primary mesh nodes, except the first two and the last two nodes, where boundary conditions are defined:

for \( r = 0 \):
\[
\phi_0 = 0, \quad \left[ \frac{\partial_h \phi_h}{\partial_h r} \right]_0 = 0,
\]

for \( r = R \):
\[
\phi_{N-1} = 1, \quad \left[ \frac{\partial_h \phi_h}{\partial_h r} \right]_{N-1} = 0.
\]

Here the difference derivative \( [\partial_h \phi_h / \partial_h r]_0 \) is approximated with the second order using three-point stencil,

\[
\left[ \frac{\partial_h \phi_h}{\partial_h r} \right]_0 = \frac{\Delta r_{1/2} + \Delta r_{1+1/2}}{\Delta r_{1/2}(\Delta r_{1+1/2} + \Delta r_{1/2})} \phi_0 + \frac{\Delta r_{1/2} + \Delta r_{1+1/2}}{\Delta r_{1/2} \Delta r_{1+1/2}} \phi_1 - \frac{\Delta r_{1/2}}{(\Delta r_{1/2} + \Delta r_{1+1/2}) \Delta r_{1+1/2}} \phi_2.
\]
For a uniform mesh with mesh step $\Delta r$ this expression simplifies to:

$$\left[ \frac{\partial_h \phi_h}{\partial \phi h} \right]_0 = -\frac{3\phi_0 + 4\phi_1 - \phi_2}{2\Delta r}.$$  

The derivative $[\partial_h \phi/\partial_h r]_{N-1}$ is approximated in the same way.

For $\alpha = 0$, the difference equation (18) is defined at the nodes $i = 1, N - 2$, except only the first and the last node of the mesh where the boundary conditions are defined,

for $r = 0$ : $\phi_0 = 0$,

for $r = R$ : $\phi_{N-1} = 1$.

The constructed difference scheme is nonlinear, i.e., it has the form of a system of nonlinear algebraic equations for solution’s nodal values. There are different ways to solve it. We employed the Newton’s method with iterations performed until the value of 2-norm of residual decreases in at least $\varepsilon = 10^{-6}$ times.

A. Series of calculations 1.

In this series of calculations, we demonstrate qualitative dependency of the solution of (30) on the values of parameters $\alpha$ and $\beta$,

$$(\alpha, \beta) \in \{0, 10^{-2}, 10^{-1}, 1\}^2.$$  

Computational domain is of the radius $R = 1$ in dimensionless coordinates. The uniform mesh with $N = 100$ nodes was used. In figure 2, the solutions of the problem are shown. We observed that for all values of parameters the corresponding solution is monotonic. Let us note that this result is not general — e.g., it is known that for generalized Fisher-Kolmogorov equation (which is equation (30) with $\beta = 0$, the mentioned properties of solution strongly depends on the values of parameter $\alpha$ and the choice of the function $f$, see, e.g., [53]).

The rows of the table in the figure correspond to the constant values of $\alpha$, its columns — to the constant values of $\beta$. The top left plot correspond to the incorrect, formal, solution of the difference scheme.

B. Series of calculations 2.

In this series of calculations we show that the solution of the problem (30) has effectively finite support as the radius of the domain increases.
Uniform mesh with \( N = 100 \) nodes was used. The parameters of the equation (30) were chosen as \( \alpha = 0.1, \beta = 0.01 \). In the figure, solutions of the problem for \( R = 1, 5, 10 \) are shown.

FIG. 2: Phase field distribution for \((\alpha, \beta) \in \{0, 10^{-2}, 10^{-1}, 1\}^2\).
FIG. 3: Phase field distribution for $R = 1, 5, 10$. Solid line is solution for $R = 10$, points — for $R = 1, 5$.

C. Series of calculations 3.

In this series of calculations, the mesh convergence was studied for the original equation, presented in [25] (which corresponds to $\alpha = \beta = 0$ here) — and for the corrected one, introduced in the current work (with $\alpha = \beta = 0.1$).

Three meshes were chosen: two uniform meshes with the number of nodes $N = 100$ and $N = 1000$, and an two adaptive meshes with logarithmic distribution of nodes. In the last case the nodal coordinates are defined as $r_i = (10^{-8})^{(N-1-i)/N}$, $i = 0, N - 1$ with number of nodes $N = 100$. In this case the minimal mesh step value at $r = 0$ is $\Delta \approx 10^{-8}$. The calculation domain is of the radius $R = 1$ in dimensionless coordinates.

In the figure [1] it is clearly seen that for $\alpha = \beta = 0.0$ when the mesh is refined, the numerical solution approaches function $\phi = 0$ in all points of $\Omega$ — except the point $r = 0$ where $\phi = 1$ and $\partial \phi / \partial r \to \infty$. In this case, the form of the numerical solutions changes significantly upon mesh refinement. That is, the numerical solution of the problem posed in [25] tends to the distribution of the order parameter with an infinitely small interface between the media, which is in consistency with the theoretical analysis of section IV. In particular, this means that the “thickness” of the diffuse boundary does not match the parameter $l$ and is never resolved by mesh.

For the regularized model mesh convergence is clearly observed even with relatively modest number of mesh points. The calculation results demonstrate mesh convergence and reflect the fact that the “thickness” of the diffuse boundary is a parameter of the model —
FIG. 4: Phase field distribution for different grids for set of parameters on the left: $\alpha = 0.0, \beta = 0.0$; on the right: $\alpha = 0.1, \beta = 0.01$

and not the numerical artifact of the computational algorithm used to solve an ill-posed boundary value problem.

VII. CONCLUSIONS

In this paper we shows that the diffuse interface electric breakdown model suggested in [25] is not completely correct from mathematical viewpoint and based on a wrong assumptions on the expression for the free energy. The source of the error appears to be a formal generalization of the diffuse fracture models to the case of the (diffuse) breakdown channel. This generalization does not take into account that codimension of the fracture mid-surface and breakdown channel are different.

Note that in [25], the simulation results are presented, which can be characterized as quite reasonable. This does not contradict the theoretical considerations, discussed above. In practice, the inconsistency of the model can be noticeable only when studying the numerical convergence of the discrete approximations of the model’s equations. Such results are not presented in any of the papers cited above, see [25–31]. Most of these papers explicitly state that the simulations were carried out using commercial software.

From the theoretical viewpoint, one can expect that using an incorrect expression for energy will result in inexistence of the $\Gamma$-limit of the diffuse interface model and the corresponding sharp interface counterpart.

Finally, the main, up to the authors opinion, conclusion that can be drawn from this work
is that, most likely, the use of high-order (“high” in the sense of “number of derivatives” or in the sense of “power of derivatives”) diffuse boundary models is the necessary when a diffuse object is, effectively, an object of codimension 2 or 3.

Although there are known (cited above) papers in which high-order diffuse interface models are considered, — their use did not have the character of a fundamental necessity. In other words, they are only quantitatively improved previously known models. For example, in the cited above work [36], the higher order model is considered as a mean to improve accuracy of isogeometric solvers.

In the case of the diffuse interface electric breakdown model considered here, the use of high-order model is a prerequisite for their mathematical correctness.

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