A mathematical model of stationary charging processes in polar dielectrics: theoretical analysis

Nadezhda Maksimova and Anna Maslovskaya
Amur State University, 21, Ignatievskoe Shosse, Blagoveshchensk, Russia
E-mail: knnamursu@mail.ru, maslovskayaag@mail.ru

Abstract. We address some global solvability issues for non-linear stationary convection-reaction-diffusion problems. Global solvability of the boundary value problem for the stationary model of a charging process of polar dielectrics under non-equilibrium external conditions is proved. The maximum principle for volume charge density is established.

1. Introduction
In recent decades, among interdisciplinary researches and applications a special place is occupied by “advection-reaction-diffusion” or “convection-reaction-diffusion” processes. This is due to the increasing role of mathematical modeling in the description of behavior of complex formalized systems as well as wide possibilities of predicting the characteristics of analyzed phenomena using techniques of computational experiment and computer simulation [1].

The deterministic approach leads to a fundamental description of convection-reaction-diffusion processes models in forms of initial-boundary value problems for parabolic partial differential equations in stationary modes and boundary value problems for elliptic equations in the case of stationary states.

“Convection-reaction-diffusion” equations can be characterized by “polyfunctionality” and employed in numerous applied fields for formalization of phenomena and processes of various nature: chemistry, biology, theory of heat and mass transfer, condensed matter physics, hydrodynamics, etc. [2–5].

This class of mathematical models also includes a drift-diffusion model of charging processes of dielectric materials under the influence of nonequilibrium external conditions. Applying the framework of this scientific area, the “drift” of charge carriers (electrons and holes) is considered, that represents an analogue of convection or advection. One of the most important particular problems is the development of a drift-diffusion approach for modeling the process of charging polar dielectrics induced by an electron irradiation [6]. This problem has been the focus of practical interests due to the need to predict the state of functional dielectrics at diagnostics and modification of their properties with scanning electron microscopy techniques. A wide range of modern studies is devoted to the development of fundamental foundations and mathematical models, the creation mathematical and software to examine charging processes in dielectrics stimulated by electron bunches [7–11].

In a series of papers (for example, [11]), techniques and methods for physical and mathematical modeling of dynamic charging processes in ferroelectric materials are presented.
We proposed a modification of the classical model of charging process for ferroelectrics taking into account the radiation-induced conductivity. Mathematically the model is described by a system of equations, including nonlinear time-dependent reaction-drift-diffusion equation to define the spatial distribution of the volume charge density, the local-instantaneous Poisson’s equation to calculate the potential distribution and the dependence between a field intensity and potential which are induced by injected charges. Since analytical solutions can be found only for certain classes of such problems, numerical methods play a significant role in the practice of computer simulation [12].

However, as the analysis suggests, if a dielectric sample is being under electron irradiation for a typical exposed time, this time is much longer, than the time of transition of the dynamic system to a stationary state (less than a microsecond). In this terms, a detailed study of mathematical models describing stationary modes becomes relevant for practice of electron microscopy.

It should be noted that a lot of attention was paid to the development mathematical models of charging effects as well as to the implementation of computational algorithms and application the special software. However, in spite of analysis of correctness of models takes a special place in the process of creating a fundamental theory of this complex phenomenon, nowadays results of theoretical studies have not been reported in the literature.

In this study, we carry out a justification of solvability of the stationary convection-reaction-diffusion problem using the mathematical apparatus described in [13]. According to this approach, the boundary value problem is represented as an operator equation. It is further proved that the equation operator is continuous, bounded, monotonous and coercive, which implies the solvability of the operator equation, and therefore of the original problem. This technique has been also applied in [14,15].

2. Statement of the boundary value problem

The mathematical model of charging processes in polar dielectrics induced by sufficiently long electron irradiation can be described by a boundary value problem for a stationary drift-reaction-diffusion equation. In a bounded domain $\Omega \subset \mathbb{R}^3$ with a boundary $\Gamma$ the following boundary value problem is considered:

$$
- d \Delta \rho + \mu_n E \cdot \nabla \rho + \frac{\mu_n}{\varepsilon \varepsilon_0} |\rho| \rho = f \quad \text{in} \quad \Omega,
$$

$$
\Delta \varphi = - \frac{1}{\varepsilon \varepsilon_0} |\rho|, \quad E = -\nabla \varphi \quad \text{in} \quad \Omega,
$$

$$
\rho = 0 \quad \text{on} \quad \Gamma.
$$

Here $\rho$ is the volume charge density, $E$ is the electric field intensity vector, $\varphi$ is the potential, $d$ is the diffusion coefficient of electrons, $\mu_n$ is the drift mobility of electrons, $\varepsilon$ is the dielectric permittivity, $\varepsilon_0$ is the dielectric constant, $f$ is the generating term responsible for the action of a volume charge source in an object.

Applying the operator $\text{div}$ to the second equation in (2), taking into account the first equation in (2) we arrive to relation

$$
\text{div} \ E = \frac{1}{\varepsilon \varepsilon_0} |\rho| \quad \text{in} \quad \Omega.
$$

Below we will refer to the problem (1), (3), (4) for given function $f$ as Problem 1.

In current paper we will prove the global solvability of the Problem 1 and the nonlocal uniqueness of its solution.
3. Solvability of the boundary value problem

Below we will use the Sobolev functional spaces \( H^s(D) \), \( s \in R \). Here \( D \) denotes domain \( \Omega \), or some subdomain \( Q \subset \Omega \), or boundary \( \Gamma \). Using \( \| \cdot \|_{s,Q} \), \( | \cdot |_{s,Q} \) and \( \langle \cdot , \cdot \rangle_{s,Q} \) we will denote norm, semi-norm, and scalar product in \( H^s(Q) \). Norms and scalar products in \( L^2(Q) \) or \( L^2(\Omega) \) we will denote respectively by \( \| \cdot \|_Q \) or \( \langle \cdot , \cdot \rangle_Q \), \( \| \cdot \|_{\Omega} \) or \( \langle \cdot , \cdot \rangle_{\Omega} \). Let

\[
Z = \{ v \in L^6(\Omega)^3 : \text{div} v \in L^6(\Omega) \},
\]

\[
H^1(\Delta, \Omega) = \{ h \in H^1(\Omega) : \Delta h \in L^2(\Omega) \}.
\]

Assume that the following conditions hold:

(i) \( \Omega \) is a bounded domain in \( \mathbb{R}^3 \) with boundary \( \Gamma \in C^{0,1} \);
(ii) \( E \in Z \), \( f \in L^2(\Omega) \).

By virtue of the Sobolev embedding theorem the space \( H^1(\Omega) \) is put into space \( L^6(\Omega) \) continuously for \( s \leq 6 \), compactly for \( s < 6 \) and with some constant \( C_s \), that depends on \( s \) and \( \Omega \), we have the estimate

\[
\| h \|_{L^6(\Omega)} \leq C_s \| h \|_{1,\Omega} \forall h \in H^1(\Omega).
\]

Bellow we will use the following Green formulas:

\[
-(\Delta u, v) = (\nabla u, \nabla v) - (\partial u/\partial n, v)_{\Gamma} \forall u \in H^1(\Delta, \Omega), \ v \in H^1(\Omega),
\]

\[
(u, \nabla v) + (\text{div} u, h) = 0 \forall u \in L^3(\Omega)^3, \text{ div } u \in L^{3/2}(\Omega), \ h \in H^1_0(\Omega),
\]

The following technical lemma holds (see [16]).

**Lemma 3.1.** Under the conditions (i), (ii), \( E \in Z \) there exist positive constants \( C_0, \delta_1, \gamma_1 \), which depend on \( \Omega \), such that the following inequalities hold

\[
| (\nabla h, \nabla \eta) | \leq C_0 \| h \|_{1,\Omega} \| \eta \|_{1,\Omega}, \ | (E \cdot \nabla h, \eta) | \leq \gamma_1 \| E \|_{L^4(\Omega)^3} \| h \|_{1,\Omega} \| \eta \|_{1,\Omega} \forall h, \eta \in H^1(\Omega),
\]

\[
| (\nabla s, \nabla s) | \geq \delta_1 \| s \|_{1,\Omega}^2 \forall s \in H^1_0(\Omega).
\]

Using the Green’s formula (7), we prove the following lemma.

**Lemma 3.2.** Let under conditions (i) \( E \in Z \), \( \rho \in H^1_0(\Omega) \) and (4) holds. Then the following relation holds:

\[
(E \cdot \nabla \rho, h) = -(\nabla h \cdot E, \rho) - (1/\varepsilon) 0)(\rho, |\rho|) \forall h \in H^1_0(\Omega),
\]

As \( h = \rho \) the relation (10) takes the form:

\[
\mu_n (E \cdot \nabla \rho, \rho) = -(\mu_n/2\varepsilon) 0)(|\rho|, \rho^2).
\]

**Proof.** Using the Green’s formula (7), we obtain

\[
(E \cdot \nabla \rho, h) = (h E, \nabla \rho) = -(\text{div}(h E), \rho) \forall h \in H^1_0(\Omega).
\]

Taking into account the following relation:

\[
\text{div}(h E) = \nabla h \cdot E + h \text{ div } E \in L^{3/2}(\Omega)
\]

and the equality (4), from (12) we arrive at (10). Setting \( h = \rho \) in (10), we obtain (11).
Let us multiply the equation (1) by a function $h \in H^1_0(\Omega)$ and integrate over $\Omega$ using the Green’s formula (6). Then we obtain the weak formulation of the Problem 1

$$d(\nabla \rho, \nabla h) + \mu_n(E \cdot \nabla \rho, h) + (\mu_n/\varepsilon\varepsilon_0)(|\rho|\rho, h) = (f, h) \quad \forall h \in H^1_0(\Omega).$$ (14)

The function $\rho \in H^1_0(\Omega)$, which satisfies (14), will be called a weak solution of Problem 1.

**Theorem 3.1.** Let $V$ is the reflexive separable Banach space. Let the operator $A : V \to V^*$ has the following properties:

1) the operator $A$ is bounded and semi-continuous, that is, for all $u, v, w \in V$ the form $(A(u + \lambda v), w)$ is continuous for $\lambda \in \mathbb{R}$;
2) the operator $A$ is monotones, that is, $(A(u) - A(v), u - v) \geq 0$ for all $u, v \in V$;
3) $A$ is continuous and bounded, which will ensure that the property

Then the mapping $A : V \to V^*$ is surjective, that is, for any $l \in V^*$ there exists such $u \in V$ that $A(u) = l$.

Let us introduce the nonlinear operator $A : H^1_0(\Omega) \to H^{-1}(\Omega)$ by formula

$$\langle A(\rho), h \rangle \equiv d(\nabla \rho, \nabla h) + \mu_n(E \cdot \nabla \rho, h) + (\mu_n/\varepsilon\varepsilon_0)(|\rho|\rho, h) \quad \forall h \in H^1_0(\Omega).$$

We show that the operator $A$ is continuous and bounded, which will ensure that the property 1) of the Theorem 3.1 is satisfied. Let the sequence $\{\rho_n \} \in H^1_0(\Omega)$ converge to $\rho \in H^1_0(\Omega)$ by norm $\| \cdot \|_{1, \Omega}$. By the Lemma 1.1 the following estimate holds:

$$|\langle A(\rho_n) - A(\rho), h \rangle| \leq dC_0\|\rho_n - \rho\|_{1, \Omega}\|h\|_{1, \Omega} + \mu_n\gamma_1\|E\|_{L^4(\Omega)^3}\|\rho_n - \rho\|_{1, \Omega}\|h\|_{1, \Omega} +$$

$$(\mu_n/\varepsilon\varepsilon_0)C_3^2(\|\rho_n\|_{1, \Omega} + \|\rho\|_{1, \Omega})\|\rho_n - \rho\|_{1, \Omega}\|h\|_{1, \Omega}. \quad (15)$$

Setting $\rho = 0$ and $\rho_n \equiv \rho$ in (15) and taking into account that $A(0) = 0$, we obtain the estimate

$$|\langle A(\rho), h \rangle| \leq dC_0\|\rho\|_{1, \Omega}\|h\|_{1, \Omega} + \mu_n\gamma_1\|E\|_{L^4(\Omega)^3}\|\rho\|_{1, \Omega}\|h\|_{1, \Omega} +$$

$$(\mu_n/\varepsilon\varepsilon_0)C_3^2\|\rho\|_{1, \Omega}^2\|h\|_{1, \Omega}. \quad (16)$$

Inequalities (15) and (16) mean continuity and boundedness of the operator $A$. Then the property 1) of Theorem 3.1 takes place.

Further, we show that for any $\rho_1, \rho_2 \in H^1_0(\Omega)$ the property 2) is valid. To this end, we subtract the relation (10) written for $\rho = \rho_2$ from (10) for $\rho = \rho_1$. We obtain

$$(E \cdot \nabla(\rho_1 - \rho_2), h) = -[(\nabla h \cdot E, \rho_1 - \rho_2) - (1/\varepsilon\varepsilon_0)(|h|_1|\rho_1| - (h, |\rho_2|_{1, \Omega})) \quad \forall h \in H^1_0(\Omega). \quad (17)$$

Setting $h = \rho_1 - \rho_2$ in (17), we arrive at relation

$$(E \cdot \nabla(\rho_1 - \rho_2), \rho_1 - \rho_2) = -(1/2\varepsilon\varepsilon_0)(|\rho_1|_1 - |\rho_2|_{1, \Omega})^2 \rho_1 - \rho_2 - \rho_1 - \rho_2)^2. \quad (18)$$

Using (18), we obtain that

$$\langle A(\rho_1) - A(\rho_2), \rho_1 - \rho_2 \rangle = d(\nabla(\rho_1 - \rho_2), \nabla(\rho_1 - \rho_2)) + (\mu_n/2\varepsilon\varepsilon_0)(|\rho_1|_1 - |\rho_2|_{1, \Omega})^2 \rho_1 - \rho_2 - \rho_1 - \rho_2. \quad (19)$$

It is clear that $d(\nabla(\rho_1 - \rho_2), \nabla(\rho_1 - \rho_2)) \geq 0$ and due to the monotony of the function $\rho|\rho|$ from (19) we arrive at the inequality

$$\langle A(\rho_1) - A(\rho_2), \rho_1 - \rho_2 \rangle \geq 0 \quad \forall \rho_1, \rho_2 \in H^1_0(\Omega)$$

that means the monotonicity of the operator $A$. 

\[ \text{doi:10.1088/1742-6596/1666/1/012030} \]
Finally, in view of (9) and (11), we obtain the inequality
\[
\langle A(\rho), \rho \rangle = d(\nabla \rho, \nabla \rho) + (\mu_n/2\varepsilon\varepsilon_0)(|\rho|, \rho^2) \geq \delta \|\rho\|^2_{1,\Omega} \ \forall \rho \in H^1_0(\Omega), \ \delta = d\delta_1. \tag{20}
\]
The inequality (20) means that the operator \( A \) is coercive and condition 3) is met.

Therefore, the Theorem 3.1 yields the solvability of the operator equation
\[
\langle A(\rho), h \rangle = (f, h) \ \forall h \in H^1_0(\Omega)
\]
and, as a consequence, the existence of a solution \( \rho \in T \) of the problem (14). For this solution, by virtue of the relation (20) the estimate holds
\[
\|\rho\|_{1,\Omega} \leq C_*\|f\|_{\Omega}, \ C_* = \delta^{-1}. \tag{21}
\]

Arguing as [15], we prove that the weak solution \( \rho \in H^1_0(\Omega) \) of Problem 1 is unique.

The following theorem holds.

**Theorem 3.2.** Assume that the assumptions (i), (ii) hold. Then there exists a unique weak solution \( \rho \in H^1_0(\Omega) \) of the Problem 1, and the estimate (21) holds.

Using some concepts of [17], let us prove maximum principle for the volume charge density \( \rho \).

Let \( f_{\text{max}} \) be a positive number and let, in addition to (i), (iii), the following condition holds:

(iii) \( 0 \leq f \leq f_{\text{max}} \) a.e. in \( \Omega \).

Arguing as [18], we prove the following lemma.

**Lemma 3.3.** Suppose that the assumptions (i)–(iii) hold. Then for the weak solution \( \rho \in H^1_0(\Omega) \) of the Problem 1 the maximum principle holds:
\[
0 \leq \rho \leq M \text{ a.e. in } \Omega, \ M = (\varepsilon\varepsilon_0 f_{\text{max}}/\mu_n)^{1/2}.
\]

Further studies are required to examine inverse problems for the model (1), (3), (4). According to the framework of the optimization approach, inverse problems will be reduced to control problems (see [19–21]). For control problems, optimal solutions can be obtained similar to the results reported in studies [21,22].

Additional studies are necessary to demonstrate the possibilities of model applications by means of numerical simulations of stationary charging characteristics obtained for typical polar dielectrics exposed to electron irradiation.

**Acknowledgments**
The authors gratefully acknowledge the support from DAAD under the Programme “Research Stays for University Academics and Scientists, 2020”.

**References**
[1] Otten D 2000 *Mathematical Models of Reaction Diffusion Systems, their Numerical Solutions and the Freezing Method with Comsol Multiphysics* (Bielefeld: Bielefeld University) p 77
[2] Kadanoff L P 2000 *Statistical Physics: Statics, Dynamics and Renormalization* (London: World Scientific Publ.) p 484
[3] Montecinos G I 2014 *Numerical methods for advection-diffusion-reaction equations and medical applications: PhD thesis* (Trento: University of Trento) p 161
[4] Kovtanyuk A E, Chebotarev A Y, Botkin N D and Hoffmann K-H 2016 *J. Math. Anal. Appl.* 439 678–89
[5] Kalmanovich V V, Seregin V V and Stepanyuk M A 2020 *J. Phys.: Conf. Ser.* 1479 012116–26
[6] Chan D S H, Sim K S and Phang J C H 1993 *Scanning Microscopy* 7 (3) 847–59
[7] Kotera M, Yamaguchi K and Suga H 1999 *Jpn. J. Appl. Phys.* 38 7176–79
[8] Raftari B, Budko N V and Vui C 2015 *J. Appl. Phys.* 118 204101–18
[9] Maskovskaya A G 2013 *J. Surf. Invest.* 7 (4) 680–84
[10] Maslovskaya A and Sivunov A V 2014 Sol. St. Phen. 213 119–24
[11] Maslovskaya A G and Pavelchuk A V 2019 J. Phys.: Conf. Ser. 1163 012009
[12] Samarskiy A A and Vabishchevich P N 2015 Numerical Methods for Solving Convection-Diffusion Problems (Moscow: LIBROKOM) p 248
[13] Lions J-L 1969 Some Methods of Solving Non-Linear Boundary Value Problems (Paris: Dunod-Gauthier-Villars)
[14] Brizitskii R V and Saritskaya Zh Yu 2016 Comp. Math. Math. Phys. 56 2011–22
[15] Brizitskii R V and Saritskaya Zh Yu 2017 Diff. Eq. 53 485–96
[16] Alekseev G V, Brizitskii R V and Saritskaya Zh Yu 2016 J. App. Ind. Math. 10 (2) 155–67
[17] Ladyzhenskaya O A and Uraltseva N N 1968 Linear and Quasilinear Elliptic Equations (New York-London: Academic Press) p 459
[18] Brizitskii R V, Saritskaya Zh Yu and Kravchuk R R 2019 Sib. El. Math. Rep. 16 1215–32
[19] Alekseev G V and Levin V A 2016 Dokl. Phys. 61 546–50
[20] Alekseev G V 2016 Diff. Eq. 52 361–72
[21] Brizitskii R V and Saritskaya Zh Yu 2018 J. Inv. Ill-Posed Probl. 9 821–34
[22] Alekseev G V 2014 Comp. Math. Math. Phys. 54 1788–803