Design of numerical algorithms for the problem of charge transport in a 2D silicon MOSFET transistor with a silicon oxide nanochannel

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Abstract. We are concerned with the problem of charge transport in a 2D silicon MOSFET transistor occupying a domain $\Omega$ with a silicon oxide nanochannel occupying a domain $\Omega_G$. After proposing an additional boundary condition for the electric potential on the common boundary of the domains $\Omega$ and $\Omega_G$ we design two numerical algorithms for funding approximate solutions of this problem. The first algorithm is a new one and uses interpolation polynomials of spline-collocation and the sweep method. The second algorithm is based on the well-known longitudinal-transverse sweep (l.t.s.) method. By using these algorithms we obtain graphs of stationary solutions of our problem. We also compare the workability and efficiency of the proposed algorithms for various values of parameters.

Introduction

By now there are plenty of mathematical models describing physical phenomena in semiconductor devices with one or another degree of reliability. For finding approximate solutions of problems of semiconductor physics we should design numerical algorithms for these models. Undoubtedly, the design of such algorithms is urgent because now semiconductor devices are essential parts of many electron appliances. The effective power and reliability of modern computers depend on features of these devices. And the main goal of mathematical modelling is to calculate all the features of a semiconductor with an accuracy requirement.

In this paper we consider a hydrodynamical model proposed recently in [1, 2]. This so-called MEP (maximum entropy principle) model is a quasilinear nonstationary system of conservation

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laws obtained from the moment system of the Boltzmann kinetic equation. It is called MEP model because for closing the moment system the maximum entropy principle (MEP) was used. The system of MEP model for the 2D case and in a dimensionless form reads

\[
\begin{align*}
R_t + \text{div}(J) &= 0, \\
J_t + \frac{2}{3} \nabla \sigma &= RQ + c_{11} J + c_{12} I, \\
\sigma_t + \text{div}(I) &= (J, Q) + cP, \\
I_t + \nabla (\alpha R) &= \frac{5}{3} \sigma Q + c_{21} J + c_{22} I.
\end{align*}
\]

(1)

Here \( R \) is the electron density, \( E \) is the electron energy, \( J = Ru, I = Rq; u = (u^{(x)}, u^{(y)}) \) is the electron velocity in the Cartesian coordinate system \((x, y)\); \( q = (q^{(x)}, q^{(y)}) \) is the energy flux, \( P = R \left( \frac{2}{3} E - 1 \right) \), \( \sigma = RE, \alpha = \frac{10}{9} E^2 \), \( Q = \nabla \phi = (\phi_x, \phi_y); \phi = \phi(t, x, y) \) is the electric potential satisfying the Poisson equation

\[
\Delta x, y \phi = \Delta \phi = \phi_{xx} + \phi_{yy} = \beta (R - \rho),
\]

(2)

and \( \rho = \rho(x, y) \) is the doping density (a given function in the domain \( \Omega \)). The coefficients \( c_{11}, ..., c_{22}, c \) of system (1) are smooth functions of the energy \( E \) detailed in [3, 4], \( \beta > 0 \) is a constant (see [5] where the reader can also find the detailed reduction of system (1) and the Poisson equation (2) to dimensionless forms). We note that in [6]–[10] various numerical algorithms were proposed for funding approximate solutions of the mathematical model (1), (2).

The present work is devoted to the construction and realization of numerical algorithms for finding stationary solutions of the problem on charge transport in a 2D MOSFET (Metal Oxide Semiconductor Field Effect Transistor). The detailed description of this semiconductor device with electron conductivity is given in [7]. Its characteristic is the presence of a silicon oxide nanochannel. The MOSFET transistor is sketched on Fig. 1 (in terms of dimensionless variables).

\begin{figure}[h]
\centering
\includegraphics[width=\columnwidth]{mosfet.png}
\caption{Schematic sketch of the 2D silicon MOSFET transistor}
\end{figure}

**Remark 0.1.** Since there is no charge transport in the nanochannel \( \Omega_G \) (see Fig. 1), in the domain \( \Omega_G \) the electric potential \( \Phi(t, x, y) \) satisfies the Laplace equation

\[
\Delta x, y \Phi = \Phi_{xx} + \Phi_{yy} = 0.
\]

(3)
The statement of the problem on charge transport in MOSFET for the equations of the MEP model is given in Section 1. Then, according to results of [8, 9], relations (1), (2) in the stationary case are rewritten as a system of three Poisson equations. For finding solutions of these equations we propose two efficient algorithms based on a nonstationary regularization, the stabilization method [11]) and the method of lines (see [12, 13]). The first of these algorithms is detailed [8, 9]. Its main idea is to approximate in the regularized equations the time derivative by a difference relation and the \(x\) derivative by an interpolation polynomial with interpolation nodes at zeros of the Chebyshev polynomial. As the result, the original problem for the equations of the MEP model is reduced to a boundary value problem for a second-order ODE system. In [9] the solution of this problem is written in the form of a cubic interpolation \(C^2\) spline. Then, we get the three point scheme

\[
\begin{align*}
\left\{ I_N - \frac{h_y^2}{6} B \right\} \hat{Y}_{k-1} - 2 \left\{ I_N + \frac{h_y^2}{3} B \right\} \hat{Y}_k + \left\{ I_N - \frac{h_y^2}{6} B \right\} \hat{Y}_{k+1} &= \\
= \frac{h_y^2}{6} \{ \mathcal{F}_{k-1} + 4 \mathcal{F}_k + \mathcal{F} \}, \quad k = 1, K - 1 \tag{4}
\end{align*}
\]

with the boundary conditions

\[
\begin{align*}
\hat{Y}_1 &= A_0 \hat{Y}_0 + B_0, \quad \hat{Y}_K = A_K \hat{Y}_{K-1} + B_K. \tag{5}
\end{align*}
\]

Here \(\hat{Y}\) is the vector of values of the unknown in the nodes of the interpolation function, \(N\) is the number of these nodes, \(I_n\) is the unit matrix of order \(N\), \(h_y\) is the mesh width of spline-interpolation; the elements of the matrices \(A_0\) and \(A_K\) and the components of the vectors \(B_0\) and \(B_K\) are determined from the boundary conditions at \(y = 0\) and \(y = 1\), and concrete expressions for the elements of the matrix \(B\) and the components of the vector \(\mathcal{F}\) are written down in [9].

Thus, the solution of the regularized equation at each time layer can be found from (4) and (5) by the matrix sweep method. Then, using the idea of the stabilization method, we pass from the previous to the next layer until the stationary solution is found. In this paper, we omit calculations towards the construction and justification of the described numerical scheme and pass at once to its realization.

There is only one serious trouble in the application of the proposed algorithm for finding solutions of the problem on charge transport in MOSFET. This is the presence of nanochannel \(\Omega_G\). However, in Section 2 under certain assumptions we give an additional mixed boundary condition for the potential \(\varphi\) on the set \(S\), where the nanochannel adjoins to the rest part of the transistor. As the result, we will be able to use the proposed numerical algorithm without any principal difficulties.

For the verification of the described methods in Section 3 we construct a second algorithm for finding numerical solutions of the boundary value problem for the Poisson equations obtained in Section 1. Here, together with the stabilization method and the nonstationary parabolic regularization we use the well-known longitudinal-transverse sweep method (this method is described in full details, e.g., in [14, 15]). Section 4 is devoted to the realization of constructed numerical algorithms. There we also detail how did we manage to get the convergence of the stabilization method, and we present graphs of obtained numerical solutions. It should be noted that we have managed to obtain solutions for any desired set of parameters of the problem only by the l.t.s. method. But, if the algorithm based on ideas from [8, 9] works for some set of parameters, then it turns out to be much more efficient than the sweep method.

1. Statement of the problem

Following [7, 16], for the mathematical model (1)–(3) we set boundary conditions (for a reason which will become clear below we restrict ourself by the statement of boundary conditions only for the potentials \(\varphi\) and \(\Phi\):
The dimensional parameter \( e \), \( L \), \( N^+ \), \( \zeta \), \( K_B \), \( T_0 \), \( P^- \), and \( n_i \) are given in Table 1. From Fig. 1 (see also (10)) we see that the doping density \( \rho \) is a piecewise constant function (in numerical computations we use some of its smooth approximations).

**Table 1. Values of the physical parameters**

| Parameter | Description                        | Value          |
|-----------|------------------------------------|----------------|
| \( e \)  | Electron charge                    | \( 1.6 \times 10^{-19} \) C |
| \( L \)  | Characteristic linear dimension    | \( 4 \times 10^{-7} \) m  |
| \( N^+ \) | Doping density in the \( n^+ \) zone| \( 10^{23} \) \( \text{m}^{-3} \) |
| \( T_0 \) | Lattice temperature                | 300 K          |
| \( K_B \) | Boltzmann constant                 | \( 1.38 \times 10^{-23} \) J K\(^{-1}\) |
| \( \zeta \) | Dielectric constant (Si)           | \( 1.03545 \times 10^{-10} \) \( \text{C} \text{m}^{-1} \) |
| \( \zeta \) | Dielectric constant (SiO\(_2\))   | \( \frac{1}{2} \zeta \) (Si) |
| \( P^- \) | Doping density in the \( P \) zone  | \( 10^{20} \) \( \text{m}^{-3} \) |
| \( n_i \) | Intrinsic electron concentration   | \( 10^{16} \) \( \text{m}^{-3} \) |
Following [9], we recall that the mathematical model (1), (2) in the stationary case can be reduced to the following system of quasilinear elliptic equations for the three unknowns $\vartheta$, $R$ and $\varphi$:

\begin{align}
\triangle \vartheta &= F^{(\vartheta)}(\nabla \vartheta, X, Q, \vartheta) = a_1|\nabla \vartheta|^2 + a_2(\nabla \vartheta, X) + \\
&\quad + a_3(\nabla \vartheta, Q) + a_4(X, Q) + a_5|Q|^2 + b \vartheta, \\
\triangle R &= F^{(R)}(\nabla \vartheta, \nabla R, Q, \vartheta, R, \varphi) = -b_1 R|\nabla \vartheta|^2 + b_2(\nabla \vartheta, \nabla R) + \\
&\quad + b_3 R(\nabla \vartheta, Q) + b_4(\nabla R, Q) + b_5 R|Q|^2 + \frac{\beta}{1 + \vartheta}(e^x - \rho)R + ncR \vartheta, \\
\triangle \varphi &= F^{(\varphi)}(\chi, \varphi) = \beta(e^x - \rho),
\end{align}

where $\vartheta = \frac{2}{3}E - 1$, $X = \frac{\nabla R}{R}$. The components of the vectors of electron velocity $u$ and the energy flux $q$ are found from the relations

\begin{align*}
u &= F(E)\{Q - (1 + \vartheta)X - F_0(E)\nabla \vartheta\}, \\
q &= G(E)\{-Q + (1 + \vartheta)X + G_0(E)\nabla \vartheta\},
\end{align*}

where $|\nabla \vartheta|^2 = \vartheta_x^2 + \vartheta_y^2$, etc.,

\begin{align*}
a_1 &= -a' F(E)F_0(E) + b' G(E)G_0(E), \quad a_2 = -1 + (1 + \vartheta)\{b' G(E) - a' F(E)\}, \\
a_3 &= a' F(E) - b' G(E) - bF(E)F_0(E), \quad a_4 = -b(1 + \vartheta)F(E), \quad a_5 = bF(E), \\
b_1 &= -m' F(E)F_0(E) + n' G(E)G_0(E), \quad b_2 = (1 + \vartheta)\{n' G(E) - m' F(E)\}, \\
b_3 &= -\frac{1}{(1 + \vartheta)^2} + m' F(E) - n' G(E) - nF(E)F_0(E), \quad b_4 = \frac{1}{1 + \vartheta} + bF(E)F_0(E), \\
b_5 &= nF(E), \quad a' = \frac{da}{d\vartheta} = \frac{3 da}{2 dE}, \quad b' = \frac{db}{d\vartheta} = \frac{3 db}{2 dE},
\end{align*}

\begin{align*}
a &= a(E) = \frac{2}{5} \frac{c_{21}}{1 + \vartheta} - c_{11}, \quad b &= b(E) = \frac{2}{5} \frac{c_{22}}{1 + \vartheta} - c_{12}, \\
m &= m(E) = \frac{c_{11} - a}{1 + \vartheta}, \quad n &= n(E) = \frac{c_{12} - b}{1 + \vartheta}, \\
F(E) &= -\frac{c_{22} - (5/3)Ec_{12}}{det}, \quad G(E) = -\frac{c_{21} - (5/3)Ec_{11}}{det}, \\
F_0(E) &= 1 - \frac{(5/3)Ec_{12}}{c_{22} - (5/3)Ec_{12}}, \quad G_0(E) = 1 - \frac{(5/3)Ec_{11}}{c_{21} - (5/3)Ec_{11}}, \\
det &= c_{11}c_{22} - c_{21}c_{12}.
\end{align*}

Thus, in the stationary case the original mathematical model (1), (2) in the domain $\Omega$ can be reduced to the system of quasilinear elliptic equations (11)–(13). To complete the statement of the problem we formulate boundary conditions for $\vartheta$ and $R$ (the boundary conditions for the
potential \( \varphi \) were given above):

\[
\begin{align*}
R &= 1, \text{ for } y = 1, \left(0 \leq x \leq \frac{1}{4}\right) \cup \left(\frac{3}{4} \leq x \leq 1\right); \\
R_y &= 0 \text{ for } y = 0, 0 \leq x \leq 1; \\
\vartheta &= 0, \text{ for } y = 1, \left(0 \leq x \leq \frac{1}{4}\right) \cup \left(\frac{3}{4} \leq x \leq 1\right), \\
\vartheta_y &= 0 \text{ for } y = 0, 0 \leq x \leq 1; \\
\left(1, \nabla \vartheta\right) &= \left(1, \nabla R\right) = 0 \text{ on } \Gamma_l, \\
\vartheta_y &= 0, \quad R_y = \frac{R}{1 + \vartheta y} \text{ on } S.
\end{align*}
\]

(14)

The boundary conditions (14) are set in the accordance of recommendations from [7, 8, 9].

There is only one trouble towards the application of the numerical method designed in [8, 9] for finding approximate solutions of the boundary value problem for \( \vartheta, R \) and \( \varphi \) in the domain \( \Omega \). This is the matching conditions (9) for the potentials \( \varphi \) and \( \Phi \). In the next section we show that under certain conditions we can redefine the boundary value problem for the potential \( \varphi \) in the domain \( \Omega \). Namely, one can formulate on the set \( S \) an additional boundary condition for the function \( \varphi \). A concrete form of this condition is determined as the result of simplification of the procedure of funding the potential \( \Phi \) in the nanochannel \( \Omega_G \).

2. Additional boundary condition for \( \varphi \) on the set \( S \)

As we can see on Fig. 1, a MOSFET transistor consists of the two parts: the domain \( \Omega \) and the nanochannel \( \Omega_G \) which adjoins to \( \Omega \) along the boundary \( S \). In the next sections we apply the numerical model from [8, 9] for funding stationary solutions of the problem of charge transport in MOSFET. But, if we try to design a numerical algorithm like that in [9] directly to equations (11)–(13) with the boundary conditions (6)–(9), (14), we have essential difficulties. The point is that in this case we have to introduce grids on the sets \( \Omega \) and \( \Omega_G \) and approximate the unknowns along the \( x \) axis by interpolation polynomials and along the \( y \) axis by a cubic \( C^2 \) spline. Then, there appears a problem with the realization of the matching conditions (9) for the spline-function as well as a number of other difficulties connected with the conformance of grid steps and sweep methods in the domains \( \Omega \) and \( \Omega_G \). In this section we propose an idea which enables one to be saved from the mentioned difficulties and perform computations only in the domain \( \Omega \). This idea is based on the smallness of the width of the nanochannel compared to its length. Starting from such an assumption we obtain an additional boundary condition on the set \( S \) for computing zero and first approximations of the potentials \( \varphi \) and \( \Phi \) in their expansions into the series in the small parameter \( \varepsilon_M \) which is the relation of the width of the nanochannel to its length. By numerical simulations using the l.t.s. method it was shown in [20] that such approximations are accurate enough.

We demonstrate the way of constructing the additional boundary condition on the example of the model problem (2), (3), (6)–(9) assuming that the function \( R \) appearing in (2) is a known function \( R(x,y) \) in the domain \( \Omega \).

**Remark 2.1.** We can simplify somewhat the model problem if instead of \( \varphi \) and \( \Phi \) we introduce the functions \( \tilde{\varphi} = \varphi - \ln \left(\frac{N^+}{n_i}\right), \tilde{\Phi} = \Phi - \ln \left(\frac{N^+}{n_i}\right) \) (below we drop tildes). Then we get the boundary condition \( \varphi = 0 \) on the drain for \( 0 \leq x \leq \frac{1}{4} \).
We now describe the procedure of finding an approximate solution of equation (3). Let us make the change of independent variables

\[ \xi = \frac{x - 5/16}{l_x}, \quad \eta = \frac{y - 1}{l_y}, \quad 0 \leq \xi, \eta \leq 1, \]

where \( l_x \) and \( l_y \) are the length and the width of the nanochannel respectively.

For the MOSFET transistor sketched on Fig. 1 the length \( l_x = \frac{3}{8} \). In terms of the new variables \( \xi \) and \( \eta \) equation (3) becomes

\[ \varepsilon_M^2 \Phi_{\xi\xi} + \Phi_{\eta\eta} = 0, \]

where \( \varepsilon_M = \frac{l_y}{l_x} \). Assuming \( \varepsilon_M \) to be small enough and dropping the first term in (16) after some transformations (see [20]) we get

\[ \varphi(x, 1) + 3l_y\varphi_y(x, 1) = G, \quad (x, 1) \in S. \]

Then, (17) is the desired additional boundary condition for the potential \( \varphi \). The potential \( \Phi(x, y) \) is found from

\[ \Phi(x, y) = 3l_y\varphi_y(x, 1)(\eta - 1) + G = [G - \varphi(x, 1)]\eta + \varphi(x, 1). \]

Thus, the boundary value problem (2), (3), (6)–(9) is reduced to the problem for the potential \( \varphi \) in the domain \( \Omega \) with the boundary conditions (6), (8a), (17). For finding an approximate solution to this problem we use the numerical algorithm designed in [8, 9] which was successfully applied for the computation of concrete semiconductor devices.

The rest of the paper is organized as follows. In the next section, basing on the well-known l.t.s. method, we construct a numerical scheme for finding approximate solutions to equations (11)–(13) and the boundary conditions (6)–(8b), (17), (14). In the last section we compare results obtained by the scheme based on the longitudinal-transverse sweep method and the algorithm which uses the numerical model from [9].

3. Longitudinal-transverse sweep method (l.t.s.)

The l.t.s. method is often used for finding numerical solutions of various nonstationary boundary value problem of mathematical physics (see, for example, [14, 15]). In this connection, it is interesting to compare the efficiency and performance of this method and the numerical scheme from [9]. We will use the l.t.s. method, which is based on difference relations approximating derivatives of unknown functions, together with the method of lines, a regularization and the stabilization method. We introduce space and time grids. The passage from the previous time layer to the next one is performed in two steps (the diagram on Fig. 2):

a) In the longitudinal sweep, going from the left boundary of \( \Omega \) to the right one along the lines \( y = y_k, k = 0, \ldots, K \) of the grid, we calculate the values of sweep coefficients by recurrence formulas. Then, we resolve the right boundary condition and in the return step (from the right to the left) we compute the unknown functions by using the found sweep coefficients.

b) In the transverse sweep, going from the lower boundary of the domain \( \Omega \) to the upper one along the lines \( x = x_j, j = 1, \ldots, N \) of the grid, we find the values of sweep coefficients. Using them and taking into account the right boundary condition, we get the values of unknown functions.

According the idea of the stabilization method (see [11]), we will perform these operations until the solution is stabilized. As the result we find a stationary solution of the problem of charge transport in MOSFET.
We now pass to the construction of the numerical model for our problem based on the l.t.s. method. This model for problem (11)–(13), (6)–(8b), (17) for a MOSFET transistor is convenient to be constructed on the example of the model problem for the Poisson equation

\[ \Delta_{x,y} \psi = \psi_{xx} + \psi_{yy} = f(x,y), \ (x,y) \in \Omega \]  

(19)

with the mixed boundary conditions

\[ \psi = \begin{cases} 
0 & \text{for } y = 1, \ 0 \leq x \leq \frac{1}{4}, \\
D & \text{for } y = 1, \ \frac{3}{4} \leq x \leq 1, \\
B & \text{for } y = 0, \ 0 \leq x \leq 1, \\
(1, \nabla \psi) = 0 & \text{on } \Gamma_1. 
\end{cases} \]  

(20)

where \( \psi \) is the unknown function and \( f(x,y) \) is a sufficiently smooth right-hand side.

Performing a parabolic regularization of the Poisson equation (19) and denoting the solution of the regularized problem by \( u(t,x,y) \), we obtain the relation

\[ u_t = \Delta_{x,y} u - f(x,y), \ u = u(t,x,y), \ t > 0, \ (x,y) \in \Omega. \]  

(21)

**Remark 3.1** By deriving a priori estimates for solutions of the original and regularized problems, it was shown in [9] that \( u(t,x,y) \to \psi(x,y) \) as \( t \to \infty \). Moreover, it was also proved there that the solution \( \psi \) of the model problem (19), (20) is asymptotically stable (by Lyapunov). This, in particular, justifies on the differential level the applicability of the stabilization method [11].
We now make time and space digitizations in equation (21). We introduce on $\Omega$ a uniform grid with the mesh points $(x_j, y_k)$ and the steps $h_x$ and $h_y$ ($j = 0, N$, $k = 0, K$, $x_j = h_xj$, $y_k = h_yk$). We consider the time grid with the mesh points $n\Delta$ and the step $\Delta$ ($n = 0, 1, 2, ...$).

Let $u = u_{jk}^n = u(n\Delta, jh_x, kh_y)$ be the mesh function

$$\Lambda = \frac{\Psi_x - 2 + \Psi_x^{-1}}{h_x^2} + \frac{\Psi_y - 2 + \Psi_y^{-1}}{h_y^2},$$

$\tau = \chi - 1$, $\chi$, $\Psi_x^{\pm 1}$, $\Psi_y^{\pm 1}$ the shift operators ($\Psi_{x,y}^{\pm 1} = \Psi_{x,y}$):

$$\chi u_{jk}^n = u_{jk}^{n+1} = \hat{u}, \quad \Psi_x^{\pm 1}u_{jk}^n = u_{jk+1}^n, \quad \Psi_y^{\pm 1}u_{jk}^n = u_{jk}^{n+1}, \quad \mathcal{F} = f_{jk} = f(x_j, y_k).$$

Then, approximating in (21) the derivatives of $u$ by difference relations, we find

$$\tau u - \Delta \cdot \Lambda \hat{u} = -\Delta \mathcal{F}$$

or

$$\hat{u}_{jk} = a(\hat{u}_{j-1,k} + \hat{u}_{j+1,k}) - b(\hat{u}_{j,k-1} + \hat{u}_{j,k+1}) = f_{jk}^n,$$

where

$$f_{jk}^n = \frac{u - \Delta \mathcal{F}}{d}, \quad a = \frac{a_x}{d}, \quad b = \frac{b_y}{d}, \quad a_x = \frac{\Delta}{h_x^2}, \quad b_y = \frac{\Delta}{h_y^2}, \quad d = 1 + 2a_x + 2b_y.$$

We will find a solution of difference relations (22) on each time layer $n = 0, 1, 2, ...$ by the l.t.s. method (see [14, 15] and fig. 2).

As the result, starting from the values $u_j^n$, we found the solution $u_j^{n+1}$ ($j = 0, ..., N$) on the $(n + 1)$th time layer. Below in Section 4 we detail the numerical scheme which gives us the stationary solution of the problem of charge transport in a MOSFET transistor by passing from a previous time layer to the next one and using the idea of the stabilization method.

4. Realization of numerical algorithms

For funding stationary solutions of the problem of charge transport in a MOSFET transistor we propose two numerical models. The first one uses the ideas from [8, 9] (interpolation polynomials of spline-collocation and the sweep method). The second one exploits the l.t.s. method and is described in the previous section. These models are based on principally different ideas, but both of them use time regularization and the stabilization method for finding stationary solutions. In this section we describe numerical schemes and details of the realizations of the algorithms constructed on the basis of the two proposed models. We also compare the efficiency of these algorithms and corresponding numerical results.

At each time layer in the process of stabilization (for both the l.t.s. method and the algorithm based on numerical model from [8, 9]) we should step by step solve three boundary value problems for the regularized Poisson equations (11)–(13). Thus, under the construction of our algorithms we first perform a regularization of equations (11)–(13). If we use the l.t.s. method, it is the parabolic regularization (21). For the technology proposed in [9] we can apply one of the two nonstationary regularizations: the parabolic or Sobolev’s one.

Remark 4.1. For example, after the application of Sobolev’s regularization to equation (19) of the model problem we get the relation

$$u_t - \Delta u_t = \Delta u - f(x, y), \quad u = u(t, x, y), \quad t > 0, \quad (x, y) \in \Omega.$$
Arguments justifying the stabilization method in the case of this regularization can be found in [9].

For numerical calculations we should define initial data \( u_0 = u(0, x, y) \).

**Remark 4.2.** To get an approximate solution for a desired set of parameters of the problem we set initial data in different ways and “pull values of parameters”. That is, we first set original initial data, for instance, such as

\[
\vartheta(t, x, y) \bigg|_{t=0} = 0, \quad R(t, x, y) \bigg|_{t=0} = 1, \quad \varphi(t, x, y) \bigg|_{t=0} = 0,
\]

and then we perform calculations for such a set of parameters that the stabilization method converges. After that as the initial data we take the obtained solution and set the values of parameters to be close to the desired ones (but so that the stabilization method converges). Then we perform calculations and again as the initial data we take the stabilized solution. Continuing such a procedure, we can finally get the stationary solution for the desired set of parameters. It should be noted that in spite of the high efficiency of the procedure of "pulling parameters" its application does not guarantee that we can find a solution for any desired range of parameters. Therefore, in numerical simulations we use this procedure together with a number of other methods (we will talk about them below).

After setting the initial data we start iterations of the stabilization method in which using the variables computed at the previous and present time layers we calculate the right-hand sides \( F(\vartheta) \), \( F(R) \), \( F(\varphi) \) and solve the equations for \( \vartheta \), \( R \) and \( \varphi \) respectively. These iterations work until the solution is stabilized, i.e., until the norm of the difference between the solutions at the next and previous time layers is close to zero. Such a numerical algorithm is described on Fig. 3.

![Diagram of numerical algorithm](image)

**Fig. 3.** Diagram of numerical algorithm

The proposed numerical algorithm was realized by Delphi 6 (Object Pascal) and Java. As input parameters the computer program took values of physical and numerical parameters of
the problem (the description of some of them is given in Table 1 above). In Table 2 we describe the set of those parameters which varied in numerical simulations.

| Parameter | Description                                      | Value     |
|-----------|--------------------------------------------------|-----------|
| $V_G$     | Gate voltage                                     | 0.36 – 1 V |
| $V_D$     | Drain voltage                                     | 0.36 – 1 V |
| $B$       | Dimensionless bulk voltage                       | -25,328 – 0 |
| $\delta$ | Dimensionless doping density in the domain $\Omega \setminus \Omega_+$ | -0.001 – 0.8 |
| $l_y$     | Width of the nanochannel                         | 1 – 20 nm  |
| $N$       | Number of mesh points along the $x$ axis         | 20 – 40    |
| $K$       | Number of mesh points along the $y$ axis         | 20 – 40    |
| $\Delta$ | Time step of the grid                            | 0.0001 – 0.1 |
| $N_{it}$  | Number of nonlinear iterations (see (23))        | 1 – 10     |
| $n_{sgla}$| Nonlinear smoothing is used after each $n_{sgla}$ steps (see (24)) | 2 – 10     |
| $\theta$ | Parameter of nonlinear smoothing (see (24))      | 0,1        |
| $\lambda$| Parameter of nonlinear smoothing (see (24))      | 1          |
| $\varepsilon_1$ | Accuracy of stabilization                       | $10^{-5}$ – $10^{-8}$ |

The algorithm stops if the necessary accuracy $\varepsilon_1$ is achieved (see [11]):

$$
\sum_{j=0}^{N-1} \sum_{k=0}^{K-1} (|R_{jk}^{n+1} - R_{jk}^{n}| + |\varphi_{jk}^{n+1} - \varphi_{jk}^{n}| + |\vartheta_{jk}^{n+1} - \vartheta_{jk}^{n}|) \leq \varepsilon_1.
$$

**Remark 4.3.** We note that in numerical simulations we aimed to obtain the stationary solution of the problem of charge transport in a MOSFET transistor for the following values of parameters (below we call these values the desired set of parameters):

$$ V_D = 1V, \ V_G = 1V, \ B = -25,328, \ \delta = -0.001, \ l_y = 20nm, \ \varepsilon_1 = 10^{-5}. $$

This set of values is a standard test (see, e.g., [7]) which is often used in real physical and numerical experiments. Finding the stationary solution for the desired set of parameters demanded some efforts.

In computations we met some difficulties. Under the usage of the stabilization method there appeared a jump growth of the unknowns caused by nonlinearity of the problem. Namely, the norm of solution became very big that led to the buffer overflow and the program stop until stabilization. To overcome this difficulty we used nonlinear iterations.

The main idea of the algorithm based on nonlinear iterations is the calculation of parameters and variables of the problem by formulas assigned for a next time layer whereas we stay at the present time layer. To clarify this we use nonlinear iterations for a modification of the scheme (4), (5). In this case the scheme (4), (5) should be reduced to the form

$$
\left\{ I_N - \frac{h_x^2}{6} B_k^{[l-1]} \right\} \hat{Y}_k^{[l]} = -2 \left\{ I_N + \frac{h_y^2}{3} B_k^{[l-1]} \right\} \hat{Y}_k^{[l]} + \left\{ I_N - \frac{h_y^2}{6} B_k^{[l-1]} \right\} \hat{Y}_{k+1}^{[l]} = \frac{h_y^2}{6} \left( F_{k-1}^{[l-1]} + 4 F_k^{[l-1]} + F_{k+1}^{[l-1]} \right), \ k = \Gamma, K - \Gamma, \ l = \overline{1, N_{it}}, \quad (23)
$$

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where the components of the vector $F_k^{[l-1]}$ and the elements of the matrix $B_k^{[l-1]}$ are calculated at the $(l-1)$th nonlinear iteration; $N_{it}$ is the number of nonlinear iterations at each time layer (see Table 2). The elements of the matrix $B_k^{[0]}$ and the components of the vector $F_k^{[0]}$ are taken from the previous time layer. At the $l$th nonlinear iteration we compute the values of the components of the vector $Y_k^{[l]}$, $k = 1, ..., K - 1$ according to (23). Then, using these values we calculate the elements of the matrices $B_k^{[l]}$ and the components of the vector $F_k^{[l]}$. After that the program passes to the $(l+1)$th nonlinear iteration. For $l = N_{it}$ we pass to the next time layer.

In numerical calculations based on the proposed algorithm there also appear short-wave oscillations of the unknowns of the problem. These oscillations precluding the convergence of the scheme with a desired accuracy have no physical meaning and are only a numerical effect. For removing these oscillations we use nonlinear smoothing. Calculations were carried out on a mesh with the points $(x_j, y_k)$ and the steps $h_x = \frac{1}{N_x}, h_y = \frac{1}{N_y}$. Let $g_j$ be the value of one of the unknowns $R$, $\vartheta$ or $\varphi$ at the point $(x_j, y^*)$, where $y^*$ is one of the horizontal lines $y = y_k$, $k = 0, ..., K$. Then the filter of nonlinear smoothing looks as follows (see [21]-[23]):

$$(g_j)_{fil} = g_j - \xi \overline{M}_{j+\frac{1}{2}} - \xi \overline{M}_{j-\frac{1}{2}},$$

where

$$\overline{M}_{j+\frac{1}{2}} = \tilde{\vartheta} g_j + \overline{N}, \quad \overline{M}_{j-\frac{1}{2}} = -\tilde{\vartheta} g_{j+1} + \overline{N},$$

$$\overline{N} = \tilde{\vartheta} g_j \overline{P} \left( \frac{\tilde{\vartheta}}{2} \tilde{\vartheta} g_j, \tilde{\vartheta} |\xi g_j|, \tilde{\vartheta} \lambda |\xi g_j|, \tilde{\vartheta} \lambda |\xi g_{j+1}| \right),$$

Here $0 \leq \tilde{\vartheta} \leq \frac{1}{2}$, $\lambda > \frac{1}{2}$ are constants (see Table 2), $\tilde{\vartheta} = \text{sign}(\xi g_j)$, $\overline{P}(a_1, ..., a_m) = \max\{0, \min(a_1, ..., a_m)\}$, $(g_j)_{fil}$ are discrete values of the component $g_j$ after the nonlinear smoothing (24). The values $\tilde{\vartheta}$ and $\lambda$ are connected by the inequality $2\tilde{\vartheta}(1 + \lambda) \leq 1$. Moreover, $(g_j)_{fil}$ and $g_j$ have the same growth direction.

The calculations using (24) were performed along each line $y^* = y_k$, $k = 0, ..., K$ (longitudinal smoothing). A filter like (24) was also used for the nonlinear smoothing of the unknown function along the $y$ axis (transverse smoothing). It should be noted that in order to absolutely remove short-wave oscillations we have to apply the filter of nonlinear smoothing after each 2–10 time steps.

In numerical calculations using the described technique, we have managed to get stationary solutions for the following sets of parameters:

a) $V_D = 0.36V$, $V_G = 0.36V$, $B = 0$, $\delta = 0.8$, $l_y = 20nm$, $\varepsilon_1 = 10^{-5}$ for the algorithm based on the numerical model proposed in [9]. The graphs for the electron energy $E$ and the electric potential $\varphi$ calculated in this case are given on Fig. 4;

b) $V_D = 0.3V$, $V_G = 0.3V$, $B = -1$, $\delta = -0.001$ $l_y = 20nm$, $\varepsilon_1 = 10^{-5}$ for the algorithm based on the l.t.s. method. The graphs for the electron energy $E$, the electron density $R$ and the electric potential $\varphi$ calculated in this case are given on Fig. 5.

However, we could not find a solution for the desired set of parameters (see Remark 4.3) because the stabilization method did not converge in this case. This trouble caused by a fast growth of the variables, the buffer overflow and the program stop prompted us to transform equations (11)–(13). To this end we introduce the auxiliary variables $\varphi^*(x, y), \tilde{\varphi}(x, y), R^*(y), \Psi(x, y)$ such that $\varphi = \varphi^* + \tilde{\varphi}$,

$$\Delta \varphi^* = \beta (R^* - \rho),$$

$$\Delta \tilde{\varphi} = \beta (R - R^*).$$

(25)
Fig. 4. Numerical results obtained by the algorithm from [9] with the parameters

\[ V_D = 0.36 \text{ V}, \ V_G = 0.36 \text{ V}, \ B = 0, \]
\[ \delta = 0.8, \ l_y = 20 \text{ nm}, \ N = 40, \ K = 30, \ \varepsilon_1 = 10^{-5} \]

Fig. 5. Numerical results obtained by the algorithm based on the l.t.s. method with the parameters

\[ V_D = 1 \text{ V}, \ V_G = 1 \text{ V}, \ B = -1, \ \delta = -0.001, \ l_y = 20 \text{ nm}, \ N = 40, \ K = 40, \ \varepsilon_1 = 10^{-5} \]
The boundary conditions for \( \varphi^* \), \( \tilde{\varphi} \) read
\[
\begin{cases}
\varphi^* = \ln \left( \frac{N^+}{n_i} \right), \; \tilde{\varphi} = 0, \; \text{for } y = 1, \; 0 \leq x \leq \frac{1}{4} \; \text{(source),} \\
\varphi^* = D, \; \tilde{\varphi} = 0, \; \text{for } y = 1, \; \frac{3}{4} \leq x \leq 1 \; \text{(drain),} \\
\varphi^* = B, \; \tilde{\varphi} = 0, \; \text{for } y = 0, \; 0 \leq x \leq 1 \; \text{(bulk);} \\
(1, \nabla \varphi^*) = 0, \; (1, \nabla \tilde{\varphi}) = 0 \; \text{on } \Gamma_1, \\
\varphi^* + 3l_y \varphi^* = G, \; \tilde{\varphi} + 3l_y \tilde{\varphi} = 0 \; \text{on } S.
\end{cases}
\]

(27)

Below we drop tildes by \( \varphi \).

In numerical calculations we used two forms of the auxiliary function \( R^*(y) \) (we tried to define it to be “close”, in some sense, to the functions obtained by cutting the graph of the given doping density \( \rho(x, y) \) by the lines \( x=\text{const} \) for \( 0 \leq x \leq \frac{1}{4}, \frac{3}{4} \leq x \leq 1 \)) by the relation
\[
R^* = R^*(y) = 3y^2 - 2y^3.
\]

(30)

Moreover, \( R^*_y = 6y(1 - y), \; R^*_{yy} = 6(1 - 2y) \). While deducing relation (30) we used the conditions \( R^*(1) = 1, \; R^*(0) = 0, \; R^*_y(0) = 0, \; R^*_y(1) = 0. \)

(31)

Here \( \kappa = \frac{7}{8} - \varepsilon_{\text{small}}, \) where \( \varepsilon_{\text{small}} << 1. \) In the deduction of (31) we started from the condition \( R^*(1) = 1, \; R^*(\kappa) = 0, \; R^*_y(\kappa) = 0, \; R^*_y(1) = 0. \) Applying (31), it is easy to calculate
\[
R^*_y = -12 \left( \frac{y - \kappa}{1 - \kappa} \right)^3 \frac{1}{1 - \kappa} + 12 \left( \frac{y - \kappa}{1 - \kappa} \right)^2 \frac{1}{1 - \kappa},
\]
\[
R^*_{yy} = -36 \left( \frac{y - \kappa}{1 - \kappa} \right)^2 \frac{1}{(1 - \kappa)^2} + 24 \frac{y - \kappa}{1 - \kappa} \frac{1}{(1 - \kappa)^2}.
\]

Remark 4.4. The cut of the doping density \( \rho(x, y) \) (see (10)) by the lines \( x=\text{const} \) for \( 0 \leq x \leq \frac{1}{4}, \frac{3}{4} \leq x \leq 1 \) has the form of a step function with the discontinuity at the point \( y = \frac{7}{8}. \) This fact was crucially used for determining the auxiliary function \( R^*(y) \) by setting the parameter \( \kappa \) (see (31)). Below we will see that the usage of such kind of function \( R^*(y) \) has proved to be very perspective for finding stationary solutions of the problem for MOSFET with the desired set of parameters.

We define the auxiliary function \( \Psi(x, y) \) by the relation
\[
\Psi = \Delta \varphi = \beta (R - R^*).
\]

(32)

Then
\[
\Delta \Psi = \mathcal{F}(\Psi) = \beta \Delta R - \Delta R^*.
\]

(33)

In the case of determining \( R^*(y) \) in the first way (see (30)) the equation for \( \Psi(x, y) \) reads
\[
\Delta \Psi = \mathcal{F}(\Psi) = \beta \mathcal{F}(R) - 6\beta (1 - 2y).
\]
If we define $R^*(y)$ in the second way (see (31)) for the unknown function $\Psi(x,y)$ from (33) we obtain the relation

$$\triangle \Psi = \mathcal{F}(\Psi) = \beta \mathcal{F}(R) + 36 \left( \frac{y - \kappa}{1 - \kappa} \right)^2 \frac{1}{(1 - \kappa)^2} + \frac{24(y - \kappa)}{(1 - \kappa)^3}. $$

The boundary conditions for $\Psi$ follow from the conditions for $R$ (see (14)):

$$\begin{cases}
\Psi = 0, & \text{for } y = 1, \quad \left( 0 \leq x \leq \frac{1}{4} \right) \cup \left( \frac{3}{4} \leq x \leq 1 \right); \\
\Psi = 0, & \text{for } y = 0; \\
\Psi_y = 0 & \text{for } y = 0, \quad 0 \leq x \leq 1; \\
(l, \nabla R) = 0 & \text{for } \Gamma_l; \\
(\Psi + \beta R^*)_y = \frac{\Psi + \beta R^*}{1 + \vartheta} (\varphi^* + \varphi)_y & \text{for } S.
\end{cases} \tag{34}$$

After above manipulations the numerical calculations are described as follows (see Fig. 6):

1. Before starting iterations of the stabilization method we should state initial data for the unknowns (see arguments in Remark 4.2) and compute the values of $\varphi^*$ by (25) with a given right-hand side.

2. In the stabilization process while solving the boundary value problems for the Poisson equation for the unknowns $\Psi$, $\varphi$, $\vartheta$ we apply one of the numerical models described above: either the model based on the l.t.s. method and described in Section 3 or the numerical model from [9]. At each time layer we step by step calculate the following functions:

   $\vartheta(t, x, y)$ by using the same relation (11) as above,
   $\Psi(t, x, y)$ by (33) (by choosing one of the two ways of determining the auxiliary function $R^*(y)$),
   $R(t, x, y) = R^*(y) + \frac{1}{\beta} \Psi$,
\( \varphi(t, x, y) \) by the formula \( \Delta \varphi = \Psi \) (see (32)).

3. We stop these operations when the norm of the difference between the solutions at the next and previous time layers becomes less than \( \varepsilon_1 \).

Performing calculations according to the above scheme, using the l.t.s. method, nonlinear iterations, the filter of nonlinear smoothing, the “pulling parameters” technique described in Remark 4.2, and defining the auxiliary function \( R^*(y) \) in the second way (see (31)), we have managed to get the stationary solution for the desired set of parameters (see Remark 4.3). The graphs for the electron density, the electron energy and the electric potential calculated in this case are given on Fig. 7.

![Graphs](image)

**Fig. 7.** Numerical results obtained by the algorithm based on the l.t.s. method with the parameters

\( V_D = 1 \text{ V}, \ V_G = 1 \text{ V}, \ B = -25,328, \ \delta = -0,001, \ l_y = 20 \text{ nm}, \ N = 40, \ K = 40, \ \varepsilon_1 = 10^{-5} \)

However, for the algorithm based on the numerical model from [8, 9] we are not able find a solution for such values of parameters. But, in the case when we take other values of parameters (e.g., \( V_D = 0,36 \text{ V}, \ V_G = 0,36 \text{ V}, \ B = 0, \ \delta = 0,8, \ l_y = 20 \text{ nm}, \ \varepsilon_1 = 10^{-5} \), see the numerical results for this set of parameters on Fig. 4), the stabilization method together with the technique described in [8, 9] converges much faster than the numerical algorithm based on the l.t.s. method.

**Conclusions**

In this paper for finding solutions of the problem on charge transport in MOSFET we proposed two efficient numerical algorithms: the algorithm using interpolation polynomials, spline approximations and the matrix sweep method, and the algorithm based on the approximation of derivatives by difference relations and the application of the longitudinal-transverse sweep method.

We hope that the obtained results stimulate a further development and improvement of numerical algorithms for problems of physics of semiconductors (this will be useful for the
construction of real devices) and the proposed methods will be adopted for finding numerical solutions of various applied problems outside semiconductor subjects.

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