

Mathematical Modeling of Water Purification Process of Iron Containing Impurities

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Abstract—This paper is devoted to mathematical modeling processes of water treatment from iron impurities. This problem is relevant for many applications, including the preparation of ultrapure water for medicine. The paper deals with a process of removing iron ions and iron oxides from water by means of a magnetic field. The two-dimensional formulation of the model problem is examined through the incompressible flow approximation in a channel with rectangular cross section. A special numerical method and parallel program were designed to solve the problem. The distributions of the concentration of the iron ions under the effect or lack of transverse magnetic field were obtained in numerical experiments.

Keywords—mathematical modeling; numerical methods; parallel algorithms; water treatment processes.

I. INTRODUCTION

This paper deals with modeling the processes of magnetic treatment of water. The processing can be applied to many industries, such as heat energetics and related industries. Water treatment of impurities and hardness salts (carbonate, chloride and sulfate salts of Ca^{2+} , Mg^{2+} , Fe^{2+} and Fe^{3+}) is used in the heat exchangers, piping and plumbing systems in various ways, including mechanical, chemical, electrophysical ones, etc. Nowadays, one of the most acute problems deals with obtaining drinking water and ultrapure water for pharmacology. For these purposes, all possibilities of water purification are used (water structuring and catching finely dispersed salts of heavy metals by a magnetic field). Magnetic water treatment is widely implemented in different industries, such as construction industry and agriculture. In the construction industry, the use of magnetic water in the hydration phase of cement processing reduces the time of solidification of cement clinker components with water. A fine-grained structure of the generated solid hydrates makes the product far stronger and increases its resistance to aggressive environmental influences [1]. In agriculture, five-hour seed soaking in magnetized water improves seed germination and can significantly increase the yield. Watering with magnetized water stimulates 15-20% growth and yield of soybean, sunflower, corn, tomatoes [2]. In medicine, the use of magnetized water helps to dissolve kidney stones and has a bactericidal effect.

It is well known that the effect of magnetic fields on water is of a complex multifactorial nature. It results in

water structure changes, its physical and chemical properties and dissolved inorganic salts behavior in water [1]. Chemical reactions in water have different speeds under the influence of amagnetic field. Magnetic treatment water softening appears to be very promising. Scale-forming salts accelerated crystallization in water occurs during such processing. This leads to a significant reduction of concentrations of dissolved ions Ca_2^+ , Mg_2^+ , and other metals. The crystals size reduction under heating is also the result of water magnetic treatment. The magnetized water can change the aggregate stability and accelerate coagulation (adhesion and sedimentation) of suspended particles with subsequent formation of finely dispersed sediment. This ability is implemented to remove sediments from water. Magnetization of water can also be applied for water supply plants with significant turbidity of natural waters. Such magnetic treatment of industrial waste water allows us to precipitate fine dirt quickly and effectively. Magnetic treatment of water helps to prevent the scale-forming salts precipitation and significantly reduces the organic substances deposits, such as paraffin. Magnetic treatment is useful for the high paraffin crude oil production. The influence of magnetic field increases provided the oil contains water.

In this work, the influence of the magnetic field on water is studied. A water stream contains ions of iron and/or iron salts ions and flows through a nonmetallic pipe. A magnetohydrodynamic model was created for this problem. The model takes into account the magnetic induction direct effect on the stream of water. In this case, the ion flux generates a secondary electric field. The paper deals with the two-dimensional plane-parallel flow. The flow is formed in the middle section of a rectangular tube with a strong anisotropy of sides. A magnetic field is applied in the transverse direction of the flow and generates circular motions in this section of the tube. In this case, the flow structure is similar to the two-dimensional model and can be seen as an initial approximation for the three-dimensional problem [3] [4]. The isothermal laminar flow of fluid is examined to simplify the analysis. The drift-diffusion approximation is used to describe the behavior of the finely dispersed impurities.

This paper is organized as follows. In Section 2, we describe the mathematical model of the problem. We then present, in Section 3, some details of the numerical algorithm. In Section 4, the main results obtained for the

steady state distribution in the stream are shown, including distribution of electrical potential, distribution of impurity concentration, and distribution of electrical field.

This paper discusses water purification of iron impurities processes. We propose some approaches to the issue in question, and finally we offer some conclusions.

II. MATHEMATICAL DESCRIPTION

An isothermal variant of water flow with impurity of iron is considered. The flow is studied in the non-conductive pipe with rectangular cross-section and with a big difference between the sizes of sides (Fig. 1).

The impurities are finely dispersed and we do not take into account the processes of association and dissociation of individual ions in clusters.

The basic equations describe water motion with impurity in the computational domain Ω [5]. This area is section $z=0$ of the original three-dimensional domain and its size is $L \times H$. The equations (1)-(3) in dimensional variables have form [6]:

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \nabla) \mathbf{u} = -\nabla p + \eta \Delta \mathbf{u}, \quad \text{div} \mathbf{u} = 0, \quad (1)$$

$$\frac{\partial n}{\partial t} = \text{div}(D \nabla n - q \mu \mathbf{F} n) + (u, \nabla n), \quad (2)$$

$$\text{div}(\varepsilon \mathbf{E}) = q(n - n_*), \quad \mathbf{E} = -\nabla \varphi, \quad (3)$$

where $\mathbf{u} = (u_x, u_y, 0)$ – velocity vector of water stream, $\rho = \rho_0 \rho(T)$ – water density at the specified temperature T , p – pressure in water stream, $\eta = \eta_0 \eta(T)$ – dynamic viscosity coefficient of water stream at the specified temperature, n_* and n – equilibrium and non-equilibrium concentrations of impurity ions in water, $D = D_0 D(T)$, $\mu = \mu_0 \mu(T)$ – diffusion coefficient and coefficient of ion mobility, q – ion charge, $\mathbf{F} = \mathbf{E} + [\mathbf{u} \times \mathbf{B}]$ – the total vector field acting on the ions, \mathbf{E} and φ – strength and potential of the electric field, $\mathbf{B} = B_0 \mathbf{e}_z$ – vector of magnetic field strength ($\mathbf{e}_z = (0, 0, 1)$), div and ∇ – operators of divergence and gradient in the spatial coordinates (x, y) , ε – dielectric constant of water.

Initial conditions (4):

$$\mathbf{u} = \mathbf{u}_0, \quad n = n_0, \quad t = 0, \quad (x, y) \in \Omega. \quad (4)$$

Boundary conditions (5) - (7):

$$x = 0: \quad u_x = u_n(y), \quad u_y = 0, \quad n = n_0, \quad \frac{\partial \varphi}{\partial x} = 0; \quad (5)$$

$$x = L: \quad \frac{\partial u_x}{\partial x} = 0, \quad \frac{\partial u_y}{\partial x} = 0, \quad \frac{\partial n}{\partial x} = 0, \quad \frac{\partial \varphi}{\partial x} = 0; \quad (6)$$

$$y = 0, H: \quad \frac{\partial u_x}{\partial y} = 0, \quad u_y = 0, \quad \frac{\partial n}{\partial y} = 0, \quad \frac{\partial \varphi}{\partial y} = 0. \quad (7)$$

At low speeds, the flow becomes stationary and can be determined by the transition to the variables ψ (current function) and ω (vortex). If we assume that the flow is irrotational, the Laplace's equation (8), (9) can be used to calculate water stream [7]:

$$\Delta \psi \equiv \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} = 0, \quad (x, y) \in \Omega; \quad (8)$$

$$u_x = \frac{\partial \psi}{\partial y}, \quad u_y = -\frac{\partial \psi}{\partial x}, \quad (x, y) \in \Omega. \quad (9)$$

The boundary conditions for the current function are expressed as follows (10), (11):

$$\psi(0, y) = \int_0^y u_n(y) dy; \quad \frac{\partial \psi}{\partial x}(L, y) = 0; \quad (10)$$

$$\frac{\partial \psi}{\partial x}(x, 0) = 0; \quad \frac{\partial \psi}{\partial x}(x, H) = 0. \quad (11)$$

The equation for the concentration can be written in form (12):

$$\frac{\partial n}{\partial t} = \text{div} \mathbf{W} + (\mathbf{R}, \mathbf{W}) + Qn, \quad (12)$$

where $\mathbf{W} = D(\nabla n - \mathbf{P}n)$, $\mathbf{P} = q\mu D^{-1} \mathbf{F}$, $\mathbf{R} = D^{-1} \mathbf{u}$, $Q = q\mu D^{-1} (\mathbf{u}, \mathbf{F})$.

For solving of the problem we used the dimensionless variables $x' = x/H$, $y' = y/H$, $t' = t/t_0$, $\psi' = \psi/u_0$, $\mathbf{u}' = \mathbf{u}/u_0$, $n' = n/n_0$, $\varphi' = \varphi/\varphi_0$, $\mathbf{E}' = \mathbf{E}/E_0$, $\Omega' = \{(x', y') \in (0, L) \times (0, 1)\}$, $t_0 = H/u_0$, $\varphi_0 = qn_0 H^2 / \varepsilon$, $E_0 = \varphi_0 / H$.

We neglect the temperature dependence of the diffusion coefficient and the mobility coefficient.

Then, the resulting formulation of the problem (13) - (15) is written as [3], [4]:

$$\Delta \psi = 0, \quad u_x = \frac{\partial \psi}{\partial y}, \quad u_y = -\frac{\partial \psi}{\partial x}, \quad (13)$$

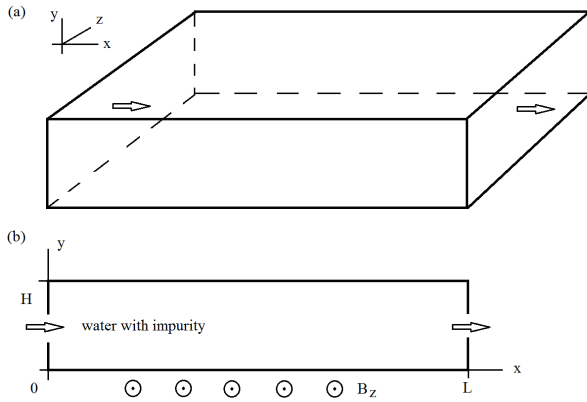


Figure 1. 3D (a) and 2D (b) computational domains.

$$\frac{\partial n}{\partial t} = \text{div } \mathbf{W} + (\mathbf{u}, \mathbf{W}) + Qn, \quad (14)$$

$$\Delta \varphi = -(n - n_*), \quad E = -\nabla \varphi, \quad (15)$$

where $\mathbf{W} = D_n (\nabla n - P_n \mathbf{F}n)$, $D_n = D_0 / (Hu_0)$, $P_n = q\mu_0 E_0 u_0^{-1}$, $Q = Q_n(\mathbf{u}, \mathbf{F})$, $Q_n = q\mu_0 E_0 HD_0^{-1}$, $\mathbf{F} = \mathbf{E} + B_n [\mathbf{u} \times \mathbf{e}_z]$, $B_n = u_0 B_0 E_0^{-1}$. The basic dimensionless parameters of the problem are: L , D_n , P_n , Q_n , B_n .

The initial conditions take the form:

$$\mathbf{u} = \mathbf{u}_0 = u_n(y) \times (1, 0), \quad n = 1, \quad u_n(y) \equiv 1 - (2y - 1)^2. \quad (16)$$

The boundary conditions for $x = 0$ (17):

$$\psi = \int_0^y u_n(y') dy', \quad u_x = u_n(y), \quad u_y = 0, \quad n = 1, \quad \frac{\partial \varphi}{\partial x} = 0. \quad (17)$$

The boundary conditions for $x = L$ take the form (18):

$$\frac{\partial \psi}{\partial x}, \quad \frac{\partial u_x}{\partial x}, \quad \frac{\partial u_y}{\partial x}, \quad \frac{\partial n}{\partial x}, \quad \frac{\partial \varphi}{\partial x} = 0. \quad (18)$$

The boundary conditions for $y = 0, 1$ are formulas (19):

$$\frac{\partial \psi}{\partial x}, \quad \frac{\partial u_x}{\partial y}, \quad u_y, \quad \frac{\partial n}{\partial y}, \quad \frac{\partial \varphi}{\partial y} = 0. \quad (19)$$

III. NUMERICAL ALGORITHM

The finite difference method is proposed to solve the problem. To do this, we introduce a uniform grid

$\Omega_h = \omega_x \times \omega_y$ in domain Ω . The grid is multiplication of 1D grids $\omega_x = \{x_i = h_x \cdot i, i = 0, \dots, N_x, h_x = L / N_x\}$ and $\omega_y = \{y_j = h_y \cdot j, j = 0, \dots, N_y, h_y = 1 / N_y\}$, where N_x , N_y – the number of network segments on x and y. We introduce also grid $\bar{\Omega}_h = \bar{\omega}_x \times \bar{\omega}_y$, where we use 1D grids $\bar{\omega}_x = \{x_{i-1/2} = 0.5(x_{i-1} + x_i), i = 1, \dots, N_x\}$, and $\bar{\omega}_y = \{y_{j-1/2} = 0.5(y_{j-1} + y_j), j = 1, \dots, N_y\}$, and uniform grid on time $\omega_t = \{t_k = \tau \cdot k, k = 0, \dots, N_t\}$ (τ – the time step, N_t – number of steps). The current function is defined on Ω_h grid (in grid nodes), other functions – on the grid $\bar{\Omega}_h$ (in the centers of the cells).

Standard differential equations are written for the current function, of the velocity vector and the potential of electric field [5][6]. They can be supplemented with boundary conditions (20), (21), if it is necessary:

$$\Lambda_h \psi_h \equiv (\psi_h)_{x\bar{x}} + (\psi_h)_{y\bar{y}} = 0, \quad (x, y) \in \Omega_h; \quad (20)$$

$$\begin{cases} u_{x,h} = +0.5(\psi_{h,y} + \psi_{h,\bar{y}}), \\ u_{y,h} = -0.5(\psi_{h,x} + \psi_{h,\bar{x}}), \end{cases} \quad (x, y) \in \bar{\Omega}_h;$$

$$\Lambda_h \varphi_h \equiv (\varphi_h)_{x\bar{x}} + (\varphi_h)_{y\bar{y}} = -(n_h - n_*), \quad (x, y) \in \bar{\Omega}_h; \quad (21)$$

$$E_h = -\nabla_h \varphi_h, \quad (x, y) \in \bar{\Omega}_h.$$

To approximate the equation for the concentration, we write it in a modified form (22), using a double integral transformation [7][8]:

$$\frac{\partial n}{\partial t} = \frac{1}{g_x} \frac{\partial}{\partial x} (g_x W_x) + \frac{1}{g_y} \frac{\partial}{\partial y} (g_y W_y) + Qn, \quad (22)$$

where $Q = Q_n(u_x F_x + u_y F_y)$, $F_x = E_x + B_n u_y$,

$$F_y = E_y - B_n u_x, \quad g_x = \exp \left[\int_0^x u_x dx' \right], \quad g_y = \exp \left[\int_0^y u_y dy' \right],$$

$$W_x = D_n \frac{1}{e_x} \frac{\partial}{\partial x} (e_x n), \quad W_y = D_n \frac{1}{e_y} \frac{\partial}{\partial y} (e_y n),$$

$$e_x = \exp \left[-\int_0^x P_n F_x dx' \right], \quad e_y = \exp \left[-\int_0^y P_n F_y dy' \right].$$

Explicit-implicit difference scheme is written, supplemented by appropriate boundary conditions (23), (24):

$$\frac{\hat{n}_h - n_h}{\tau} = \bar{\Lambda}_h \hat{n}_h + \bar{Q}_h \hat{n}_h, \quad n_h|_{t=0} = 1, \quad (23)$$

$$\bar{\Lambda}_h \hat{n}_h = \frac{1}{g_{x,h}} \left((g_{x,h} W_{x,h})_x \right)_{\bar{x}} + \frac{1}{g_{y,h}} \left((g_{y,h} W_{y,h})_x \right)_{\bar{x}}, \quad (24)$$

where $g_{x,h} = \exp \left[\sum_{0 \leq x' \leq x} u_x h_x \right]$, $g_{y,h} = \exp \left[\sum_{0 \leq y' \leq y} u_y h_y \right]$,

$$W_{x,h} = D_n \frac{1}{e_{x,h}} (e_{x,h} n_h)_x, \quad W_{y,h} = D_n \frac{1}{e_{y,h}} (e_{y,h} n_h)_y,$$

$$e_{x,h} = \exp \left[- \sum_{0 \leq x' \leq x} P_n F_{x,h} h_x \right], \quad e_{y,h} = \exp \left[- \sum_{0 \leq y' \leq y} P_n F_{y,h} h_y \right].$$

The implementation of schemes is performed by using iterative algorithms of alternating directions [9] and methods of non-monotonic sweep.

The parallel realization of the algorithm is based on the methods of domain decomposition [10] [11], and [12] and a sweep parallel algorithm. Computer implementation is performed by using Message Passing Interface (MPI) and Open Multi-Processing (OpenMP) technologies [13], [14].

There are both advantages and disadvantages of the proposed mathematical approach.

Firstly, the proposed model, of course, is incomplete because it does not take into account the reverse influence of changes of the ions concentration on flow characteristics. However, in many cases, these corrections are of little significance. At the same time, the rejection enables us to calculate relatively easily the basic process of an electromagnetic treatment of water.

Secondly, the transition to the current function enables us not to worry about condition $div \mathbf{u} = 0$, that (in alternative numerical algorithms) is a big problem.

Thirdly, the rejection of the calculation of the vortex structure of flow at low speeds does not have much value, but saves computation time.

Fourthly, the use of staggered grids enables us to reduce errors during interpolation of solution from one grid to another.

Fifthly, the application of exponential schemes releases from the problem of stability of the solution equation algorithm for the concentration and separation of boundary layers. Of course, the implementation of an exponential scheme increases the computation time. However, this increase is not catastrophic and can be compensated by using parallel computing.

Thus, the proposed approach has the following advantages: low time-consuming and highly stable calculations.

IV. COMPUTATIONAL RESULTS

In this section of the paper, the data on numerical experiments are described. To test the numerical algorithm, we chose the calculation variant with values of the dimensionless parameters $L = 6$, $D_n = 1$, $P_n = 1$, $Q_n = 1$, $B_n = 1$. Grid parameters are equal: $N_x = 300$, $N_y = 50$, $h_x = h_y = 0.02$, $\tau = 10^{-4}$.

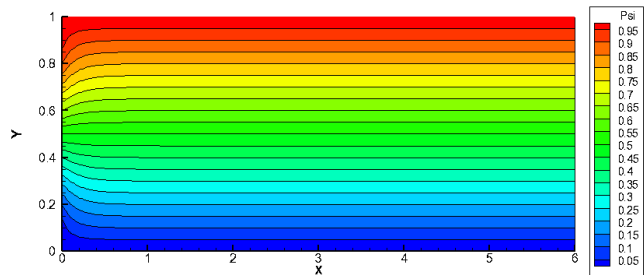


Figure 2. The stream function distribution in the computational domain.

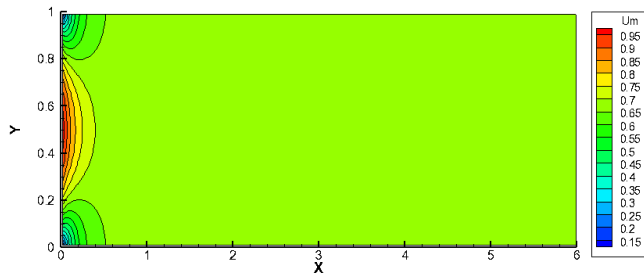


Figure 3. The velocity modulus distribution in the computational domain.

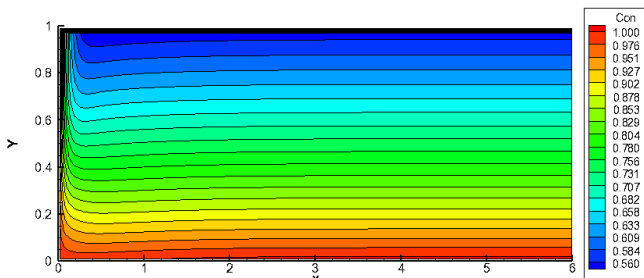


Figure 4. The steady state distribution of impurity concentration.

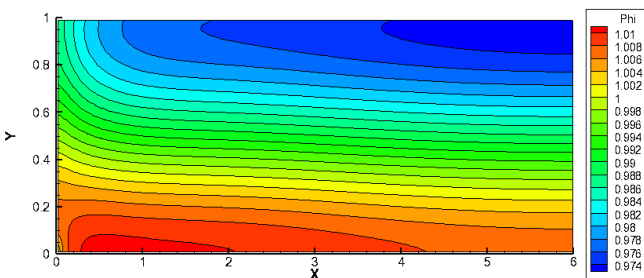


Figure 5. The steady state distribution of electrical potential.

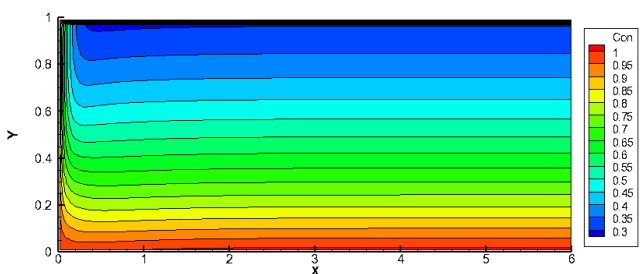


Figure 6. The steady state distribution of impurity concentration for $B_n = 2$.

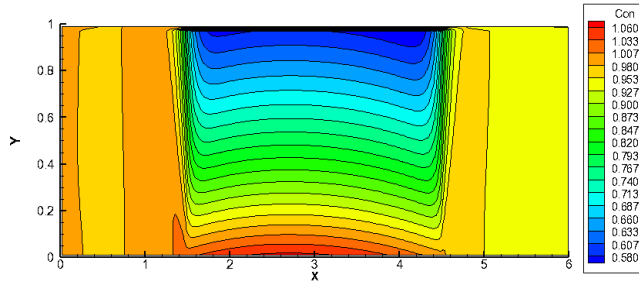


Figure 7. The steady state distribution of impurity concentration into and near localized area for $B_n = 1$.

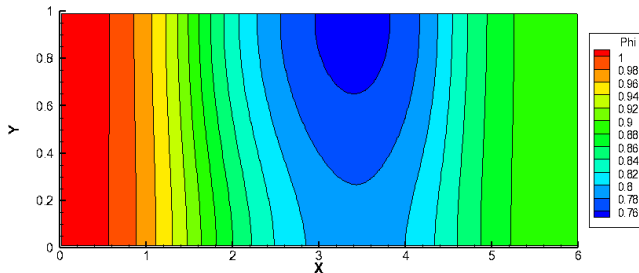


Figure 8. The steady state distribution of electrical potential into and near localized area for $B_n = 1$.

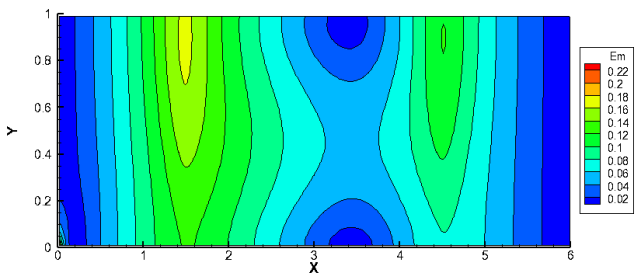


Figure 9. The steady state distribution of electrical field into and near localized area for $B_n = 1$.

The results of calculations are shown in several figures. Fig. 2 presents the stream function distribution in the computational domain. The velocity modulus distribution in the computational domain is displayed in Fig. 3. The steady state distribution of impurity concentration is given in Fig. 4. We can estimate the distribution of electrical potential from Fig. 5.

Analysis of the data shows the following. The influence of the magnetic field leads to decreasing ions concentration at the top of the area for positive values of B_n parameter and formation of increased ion concentration at the bottom layer. Thus, the purification effect of the upper liquid layer is realized.

The value of cleaning depends on the B_n parameter. It becomes noticeable when the Lorentz force is comparable to the hydrodynamic pressure forces, that is $B_n = 1$. Our executed calculations show that reduction of impurity concentration is achieved approximately 2 times for $B_n = 1$.

If parameter $B_n = 2$, the reduction of impurity concentration at the upper liquid layer is about 3.5 times (Fig. 6).

The space localized effect of magnetic field is implemented in industrial purification systems. In our work, we introduce B_n parameter dependence on the longitudinal coordinate x . For example, we consider a localization of a magnetic field in the area $x \in [1.5, 4.5]$ and value $B_n = 1$. The calculation results are presented in Fig. 7 and Fig. 8. They show that the layer of purified water is situated in the upper part of the localized area. Water taking may be done from the region, for example, through a special membrane. The steady state distribution of electrical field into and near localized area for $B_n = 1$ is shown in Fig. 9.

V. CONCLUSIONS

The issue of water purification of iron impurities by means of electro-magnetic methods is discussed in this paper. A simplified mathematical model was developed for the model problem, describing the the purification process. A numerical algorithm was proposed and the parallel code was constructed for computer experiments. Tests of the code with various sets of parameters confirmed the operability of the proposed computational approach.

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