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Mathematical modelling of physical processes in thin pre-electrode layer of a magnetic colloid.

NATALYA KANDAUROVA[1], VLADIMIR CHEKANOV[2],
VLADIMIR KANDAUROV[1]

Abstract

The material of the paper deals with the Mathematical modelling of physical processes. Using the perfect computer technologies the described mathematical model of autowaves in the pre-electrode layer of magnetic colloid is based on the differential equation in private derivatives of parabolic type with two spatial variables.

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The Present stage of development of a science is characterized by research of a various sort of the nonlinear phenomena. However by present time wave processes self-supported in the active nonlinear environment are known not many, which could be observed experimentally for small (the order of 1 minute) period of time and which parameters could be changed in laboratory conditions. The mathematical model of such process consists of the limited number of the equations, i.e., on the one hand, is simple enough, and with another, enables to describe and understand the big circle of the complex phenomena. Pre-electrode layer of magnetic colloid (a magnetic liquid), placed in electrophoresis cell, at influence of an electric field represents such active nonlinear environment in which autowave process (aw-process) [1] was observed. Mathematical modelling of autowaves in electrophoresis cell with a magnetic liquid and the numerical decision of the equation of autowaves is in our opinion a rather interesting problem. For the solving a task with numerical methods of the solving of the nonlinear differential equations, descretization of areas and the approximation of dependences included in mathematical packages MathCad, MatLab and Curve Fitting Toolbox 1.1.1, COMSOL Multiphysics were used.

[1] *Department of information systems and technology, North-Caucasian State Technical University, Kulakov 2, Stavropol, 355029, Russian Federation (candaur@stavropol.net)*
[2] *Stavropol State University Pushkin 3,Stavropol, 300017, Russian Federation (candaur@stavropol.net)*

The described mathematical model is based on the differential equation in private derivatives of parabolic type with two spatial variables:

$$\frac{\partial \rho_s}{\partial t} + D\left(\frac{\partial^2 \rho_s}{\partial x^2} + \frac{\partial^2 \rho_s}{\partial y^2}\right) = j(t),\ \ x \in (0, l_1),\ \ y \in (0, l_2),\ \ t > 0, \tag{1}$$

where ρ_s – The maximal charge, relied to unit of a surface; D – diffusion coefficient; $j(t)$ – The vector of density of a current is directed perpendicularly to settlement surface.

The nonlinear differential equation (1) can be solved analytically only for stationary autowaves (the automodelling decision) provided that and $\tau_1 1$ - time of recreation is much more than $\tau_2 2$ - time of excitation.

For the numerical decision of an initial problem completely implicit differential scheme is applied. The uniform existential grid is entered on rectangular area:

$$G = \{(x_i = i\Delta x,\ y_i = j\Delta y,\ t = k\Delta t),|\ i = 0,1,...,n,\ j = 0,1,...,m,\ k = 0,1,...,s\} \tag{2}$$

The boundary and entry conditions of the first order are set:

$$\begin{aligned} &\rho_s(x,0,t) = f_1(x,t),\ \ x \in [0,l_1],\ y = 0,\ t > 0; \\ &\rho_s(x,l_2,t) = f_2(x,t),\ \ x \in [0,l_1],\ y = l_2,\ t > 0; \\ &\rho_s(0,y,t) = f_3(y,t),\ \ x = 0,\ y \in [0,l_2],\ t > 0; \\ &\rho_s(l_1,y,t) = f_4(y,t),\ \ x = l_1,\ y \in [0,l_2],\ t > 0; \\ &\rho_s(x,y,0) = \psi(x,y),\ x \in [0,l_1],\ y \in [0,l_2],\ t = 0. \end{aligned} \tag{3}$$

Discretizing the equation (1) for internal points of a grid:

$$\frac{\rho_{i,j,k} - \rho_{i,j,k-1}}{\Delta t} + D\cdot(\frac{\rho_{i+1,j,k} - 2\rho_{i,j,k} + \rho_{i-1,j,k}}{(\Delta x)^2} + \frac{\rho_{i,j+1,k} - 2\rho_{i,j,k} + \rho_{i,j-1,k}}{(\Delta y)^2}) = J_{i,j,k}, \tag{4}$$

where $i = 2,...,n-1; j = 2,...,m-1; l = 2,...,s-1$ and writing the equation (4) for all elementary cells of area of integration, we come to system from the algebraic equations with the unknown members . The system (4) is characterized by a five-diagonal matrix. In a bidimentional case the decision of a problem (1) under corresponding regional conditions is reduced to finding on each time layer of the solving a system of the algebraic equations with a five-diagonal matrix. For check of convergence of the constructed computing scheme its order of approximation on time and to spatial variables has been found and stability is investigated. It is proved, that differential scheme which was used is absolutely steady and approximates an initial problem with the first order of accuracy on *t* and with the second order of accuracy on *x, y.*

As the optimal equation for the solving of autowave process the method of final elements which allows to consider inconstancy of parameters inside of elements of considered system and existing nonlinearity has been chosen, and as the tool of research the complex of tool means of technology of scientific modelling - COMSOL Multiphysics has been used.

The numerical decision of the equation of autowave process (1) has been found with use of two products of software:

1. The interactive environment for modelling and the decision of the differential equations in private derivatives COMSOL Multiphysics in which the technology of final elements is applied.

2. Mathematical package MatLab 6.5 with program realization of algorithm of a numerical method. The estimation of productivity of the decision (time of calculation) the equations of autowave process enables more obviously to see an optimality of application of a method of final elements in comparison with a grid method.

In the equation (1) autowave process is caused by presence of nonlinear composed *j (t)* (fig. 1)

Under the schedule on fig. 1 it is visible, that dependence $j(t)$ includes two components $j^{(1)}(t)$ and, $j^{(2)}(t)$ where $j^{(1)}(t)$ - the current of a charge describing a phase recreation, $j^{(2)}(t)$ - the current of the category describing a phase of excitation of autowave process. The current of a charge consists of two composed: $j^{(1)}(t) = j_1^{(1)}(t) + j_2^{(1)}(t)$, where $j_1^{(1)}(t)$ - adsorption current caused by accumulation of a free charge on an interface of layers, - a $j_2^{(1)}(t)$ is an residual current or the current of conductivity caused only by passing conductivity.

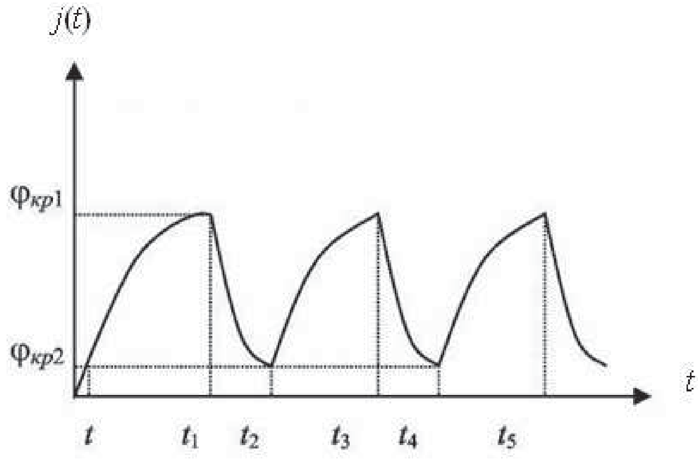

Figure 1 - Dependence of density of a current on time

j (t) is explosive function on the first derivative, therefore for the solving of the equation (1) its smoothing by means of program MatLab 6.5 has been lead. The result of the numerical decision of the equation (1) in COMSOL Multiphysics environment is presented on fig. 2.

From fig. 2 it is visible, that value of required size and ρ_S - the maximal charge carried to unit of a surface, changes within the limits of from 8·10-5 up to 1·10-3 Cl/m^2, that will be coordinated with experimental data [2], [3], [4].

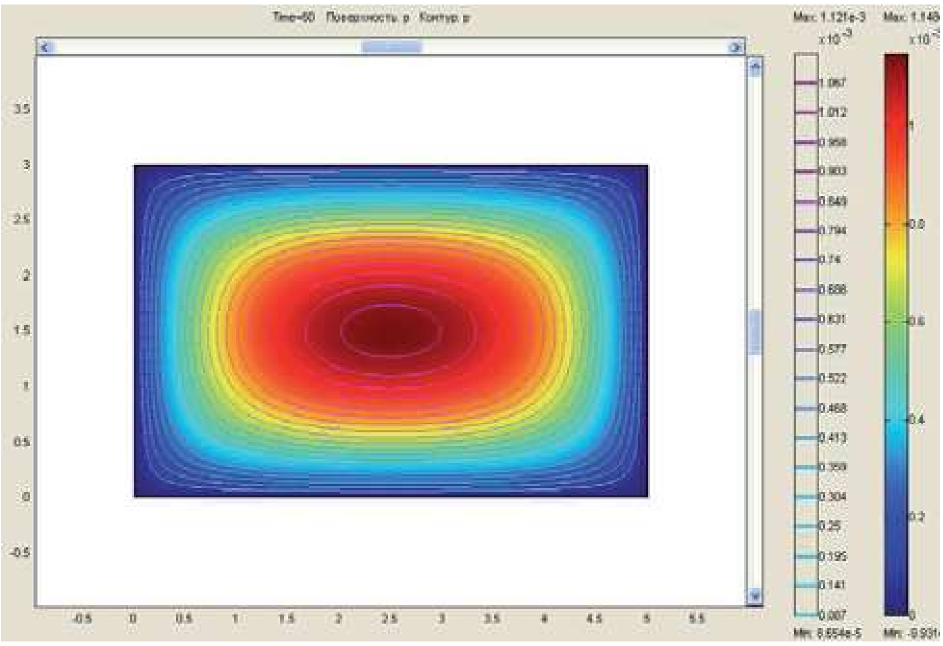

Figure 2 - Value of size of the maximal charge carried to unit of a surface, calculated in COMSOL Multiphysics environment

In mathematical MatLab 6.5 environment the program of visualization of the numerical decision of the equation of autowave process (fig. 3) has been developed.

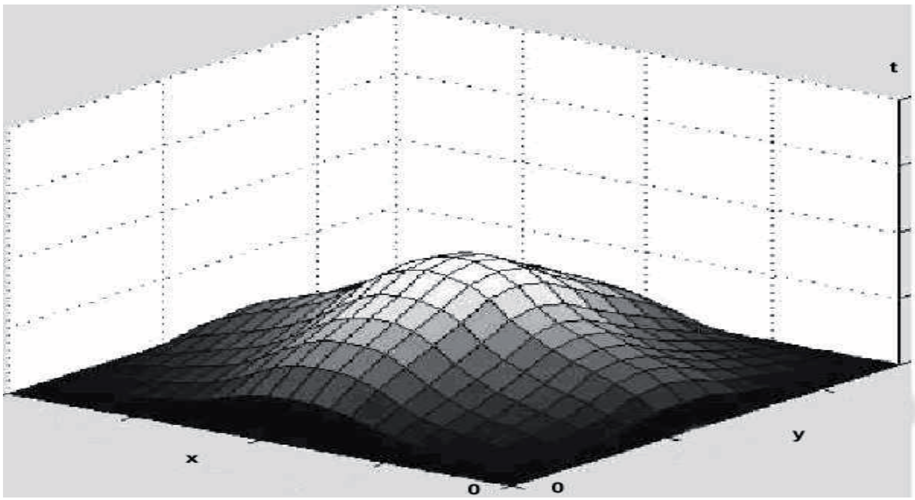

Figure 3 - Visualization of dynamics distribution of a charge and ρ_S on a surface electrophoresis cells

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Natalya Kandaurova North-Caucasian State Technical University,
Vladimir Chekanov Stavropol State University
Vladimir Kandaurov North-Caucasian State Technical University,

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