Mathematical modeling of the autowave diffraction process in a cell with a magnetic fluid

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Abstract. In this work, we simulate the diffraction of autowaves propagating in the near-surface layer of a magnetic fluid. As a basis for the model being developed, the FitzHugh-Nagumo base model is used. A solution is obtained in the COMSOL Multiphysics physical process modeling environment.

1. Introduction
A large number of works have been devoted to the problems of self-sustained waves in active medium. Starting with the fundamental work of A.N. Kolmogorov, I.G.Petrovsky, N.S. Piskunov in 1937 and up to the modern works of M.Tsiganov, T.K.Starozhilova, G.R. Ivanitsky, A.Mikhailov, K.I. Agladze and other authors. Interest in this topic is due primarily to the fact that the laws of behavior and propagation of autowaves are the same and are used to explain phenomena in biology, chemistry, medicine, urbanistics and other fields.

According to I.R. Prigozhin’s definition, autowaves are self-sustained excitation waves in an active medium, which retain their characteristics as constant due to energy sources distributed in the medium.

The authors of [1,2,3,4] have established that the near-electrode thin layer of a nanostructured colloidal medium - a magnetic fluid [5] - is an active one. In the electric field, after the voltage at the electrodes exceeded the threshold value, an autowave process and all its typical phenomena were observed: pacemakers, reverberators, annihilation in a collision.

One of the properties of autowaves is their ability not to be reflected from obstacles, but to change the direction of propagation and speed near the obstacle, and, as a consequence, to bend it.

This phenomenon, in our opinion, has not been sufficiently studied, but at the same time it is of practical interest, so this situation can actually take place in the cardiac muscle, when the period of refractoriness of individual parts of the myocardium increases due to the necrosis of tissue in a heart attack.
The description of experiments on the autowave process observation in the near-electrode layer of a magnetic fluid can be found in [1-3].

The purpose of this article is to study the autowave diffraction in the near-electrode thin layer of a magnetic fluid with obstacles of various shapes, to create a mathematical model for this phenomenon and to realize this model in a computer experiment, making a comparison of the results with full-scale experiment.

2. Experimental
The magnetic fluid used in the experiments is a colloidal solution of magnetite particles with a radius of about 10 nm in kerosene. The particles have a shell of surfactant (oleic acid), which prevents their coagulation. A magnetic fluid is placed between two transparent electrodes, which is an ITO layer deposited on the glass. In an electric field, magnetite particles migrate to the electrodes and form thin layers near them. Between the particle layer and the electrode there is a thin layer of dielectric (probably a mixture of kerosene and oleic acid), the so-called structural-mechanical barrier that prevents the particles and the electrode from coming into contact. Its thickness is \( \sim 30 \mu m \). The barrier is formed due to adsorption of the surfactant both on the particle surface and on the surface of the electrode.

The scheme of the experiment is shown in Figure 1. Electrodes are supplied with a voltage (constant or pulsed).

Let \( U \) be the voltage at the electrodes, \( E \) – field strength between the layer of magnetic fluid particles (2) and the electrode ITO (4). When the voltage reaches a certain threshold value \( U_{cr} \), the strength in a thin dielectric layer reaches \( E \sim 10^7 \text{ V/m} \).

With such a strength, the layer resistance decreases sharply, it becomes conductive, the chemical equilibrium constant changes sharply, the concentration of ions increases significantly.

The second effect of Wine takes place: the equilibrium in a strong electric field shifts toward the formation of ions.

![Figure 1. Schematic of a cell with a magnetic fluid with a formed near-electrode layer, 1 - magnetic fluid in the cell, 2 - a layer of magnetite particles, 3 - dielectric (structural-mechanical barrier), 4 - electrode (ITO)](image)

The particles of the near-electrode layer get the same sign charge with the electrode and start moving from the electrode to the region with a low-concentration liquid (1), where they are quickly discharged (discharge time \( \sim 10^{-3}\text{s} \)). The near-electrode layer collapses.
Those particles, which fall into a region with a low-concentration liquid lose their charge, get oppositely charged, and begin to move to the electrode again. The process repeats, brightly colored autowaves can be visually observed on the electrode surface. The method of autowave process observing is described in [1].

The physical meaning of the model lies in the fact that a system of coupled nonlinear oscillators is considered.

Since autowaves, in contrast to other types of waves (mechanical, electromagnetic), do not carry energy with them, but use the energy of the autowave medium, then in the near-electrode layer of particles there must be a large number of local elements (sections of the layer), each of which has its own energy source and can be in one of three states: peace, refractoriness or excitement. It accumulates energy, like a capacitor, and works as an autonomous energy source. Each such region is a non-linear oscillator, and the entire medium is a system of coupled relaxation oscillators.

After passing the autowave pulse, the active medium restores its properties due to the energy coming from outside.

The time necessary for its recovery is called the refractory period. During the refractory period, the medium is not capable of carrying out the next pulse.

The autowave process has two types fast and slow. The fast process corresponds to the discharge of the capacitor, the slow process corresponds to the charge.

The same type of description of autowave phenomena of a different nature consists in the fact that they are all described by parabolic partial differential equations with a nonlinear free term.

3. Theory and calculation

To simulate spiral waves, we use the basic FitzHugh-Nagumo model, which describes an autowave process in excitable medium. It allows to adjust the parameters of the autowave process widely and change the characteristics of its flow.

The model consists of two equations, the first equation describes a fast process – a change in the intensity in the near-electrode layer after the increase in the conductivity of the structural-mechanical barrier.

The second equation describes a slow process the change in charge of the near-electrode layer, when charged particles of magnetite accumulate in it.

\[
\frac{\partial V}{\partial t} + \frac{\partial^2 V}{\partial x^2} = D\Delta V - V^3 + V - I; \\
\frac{\partial I}{\partial t} = \varepsilon(V + \alpha - bI)
\]  

(1)

\(V\) – function, depending on the field intensity in a thin near-electrode layer of a magnetic fluid (activator);

\(I\) – function associated with a change in charge (inhibitor);

\(D\) – diffusion coefficient of the activator;

\(\varepsilon\) – a small parameter, presumably this is the ratio of the time of single pulse passage and the time of the near-electrode layer formation;

Depending on the values of the parameters \(\alpha\) and \(\beta\), the medium element can be either in the autooscillatory mode or in the excitable mode. In the case of an excitable medium, oscillations arise due to feedback, which is provided by periodic boundary conditions [6].

Numerical experiments were carried out using the finite element method, which is the basic for the COMSOL Multiphysics 5.2 and its General Form PDE.

Based on the results of the full-scale experiment, the following modification of the FitzHugh-Nagumo system was obtained:
\[
\frac{\partial V}{\partial t} + \frac{\partial^2 V}{\partial x^2} = \frac{(\alpha - V)(V - 1)V - I}{1 + 2\phi};
\]

\[
\frac{\partial I}{\partial t} = \varepsilon (1 + \frac{\phi}{1.5})(\beta V - \gamma I - \delta)
\]

The coefficients \( \beta, \gamma \) and \( \delta \) are chosen for the stability of the system and the creation of the required waveform. In this case we may ignore the activator diffusion.

The coefficients \( \alpha \) and \( \varepsilon \) are responsible for the properties of the medium and have the following meaning: \( \alpha = 0.01 \) - excitation limit, \( \varepsilon = 0.005 \) - excitability, that is, the ratio of the times of fast and slow processes.

The initial conditions are set depending on what the model should represent. For example, a circular reverb is specified by the conditions:

\[
V = V_0(x > x_0)(y > y_0)
\]

\[
I = I_0 \tanh(80(y - y_0))
\]

Where \( V_0 \) and \( I_0 \) are the initial values of the functions \( V \) and \( I \) (1 and 0.3, respectively), \( x_0 \) and \( y_0 \) are the coordinates of the reverberator center.

For radial groups of reverberators, the initial conditions are:

\[
V = V_0((\sin(\arctan 2(y, x)N)))
\]

\[
I = I_0(\cos(\arctan 2(y, x)\frac{N}{2} - 0.25))^4
\]

where \( N \) is the number of reverberators.

In addition to the coefficient \( \phi \), the zero boundary condition of the zero flux is used on all geometric boundaries of the cell:

\[-\alpha = 0\]

4. Results and discussion

The model was implemented in the form of computer simulation. The resulting solution for an autowave process with obstacles is shown in Figure 2:

The problem to determine the change in the speed of an autowave near an obstacle and to determine the nature of the change in autowave propagation conditions at an obstacle, depending on the deceleration parameter \( \phi \).

To determine the influence of the parameter \( \phi \) on the properties of the wave, a simulation with the following parameters was carried out:

The deceleration parameter \( \phi \) was given by the equation:
Figure 2. Results of a computer experiment. Distribution of the inhibitor value along the plane of the near-electrode layer.

\[ \phi = \frac{(\tanh(-0.02 - y) \cdot 0.045 + 2)}{2} + 0.05 \]  

Equation (3) was written taking into account the result of full scale experiments. That is, the reverse problem was solved: the results of simulation should be consistent with the experimental data, as a criterion of the adequacy of the used model.

The nature of the change in the parameter \( \phi \) is shown in Figure 3.

The figure shows that the deceleration parameter \( \phi \) varies nonlinearly, depending on the distance from the obstacle.

Figure 3. Changing the deceleration parameter \( \phi \): a) the distribution of \( \phi \) in the modeling area; b) Dependence of \( \phi \) on the coordinate (distance from the obstacle)

The wavelength \( \lambda \) was measured on the inhibitor distribution graphs (Figure 4) along the central vertical line from \((0, -0.05)\) to \((0, 0.05)\), the period \( T \) is shown in the graph of the inhibitor and activator in time at a single point in the lower part of the cell. The values were measured over 6-7 autowave periods and were averaged to improve the accuracy of the results.
The results for determining the dependence of the autowave properties on the deceleration parameter $\phi$ are presented in Table 1. The velocity was calculated by the formula: $V = \frac{\lambda}{T}$.

Table 1. Autowave parameters.

| Deceleration parameter $\phi$ | Wavelength, mm | Frequency, Hz | Speed, mm/s |
|------------------------------|----------------|---------------|-------------|
| 0                            | 9.91           | 0.003247      | 0.032175    |
| 0.1                          | 9.41           | 0.003192      | 0.030035    |
| 0.2                          | 8.71           | 0.003229      | 0.028124    |
| 0.3                          | 7.47           | 0.003372      | 0.025185    |
| 0.4                          | 6.67           | 0.003463      | 0.023096    |
| 0.5                          | 6.13           | 0.003726      | 0.022839    |
| 0.6                          | 4.96           | 0.003858      | 0.019136    |
| 0.7                          | 4.66           | 0.003888      | 0.018118    |
| 0.8                          | 3.66           | 0.00392       | 0.014347    |

Since the model is qualitative, not quantitative, units of measurement are considered conditional. A dependence graph of the autowave velocity on the deceleration parameter $\phi$ is shown in Figure 5.
As can be seen from the graph, the velocity decreases linearly with increasing coefficient $\phi$. Let us now consider the dependence of the change in the velocity of the wave from the distance to the obstacle (Figure 6).

Figure 6 shows that the velocity dependence on distance to the obstacle is nonlinear. The rapid loss of speed of the autowave near the obstacle allows the outer part of the wave to overtake it, so the diffraction (or bending) of the autowave occurs.
The obtained results of the simulation are in good agreement with the full-scale experiment shown in Figure 7. This proves the correctness of the presented mathematical model.

Figure 7. Autowave diffraction at obstacles of various shapes. Full-scale experiment

5. Conclusions
1. Based on the FitzHugh-Nagumo basic model (FHN), a mathematical model of the autowave diffraction on obstacles of different shapes has been developed.
2. The model is implemented in the interactive system for modeling physical processes COMSOL Multiphysics.
3. The coefficients in the equations of the modified FitzHugh-Nagumo model are found, for which the qualitative parameters of the model correspond to the experimental ones, the wave velocity is calculated for propagation in the region of the changed parameters.
4. It is shown that the diffraction of autowaves (deflection of obstacles) is a consequence of the existence of a region with non-linear characteristics near obstacles. One of the characteristics is the deceleration parameter $\phi$. An equation specifying this coefficient is written.
5. Introduction of the deceleration parameter in the mathematical model allows obtaining simulation results that are in good agreement with the full-scale experiment.

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