On the Modeling Ion Motion in Electromagnetic Field

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Abstract—**The approach to the study of influence of low frequency and low intensity electromagnetic fields on living organism in medical practice is considered. It is based on approximate calculation of magnetic field in given points of the space and modeling the motion of ions under action of the field. We present the imitation model of this motion with visualization of results in ParaView package. The proposed tool may be useful both for designers of magnetoterapy devices and physicians using such devices in practice.**

Keywords—magnetic and electric fields; magnetoterapy; ion motion; mathematical models

I. INTRODUCTION

It is well known that physical fields of different intensities actively influence on living organisms functioning. The part of biophysics called magnetobiology studies biological effects of mainly weak static and low-frequency magnetic fields on the biological systems at all levels: molecular, cellular, and whole organism. This area of science develops successfully last 15-20 years and accumulated significant amount of data. The detailed review one may find in [1]. In medicine effects of electrical and magnetic fields well complement traditional medicine treatment.

It should be noted that in spite of wide-spread practice of using magnetotherapy devices, up to now there is no common rules for their parameters choice. First of all, it is connected with the fact that the action of low intensities electromagnetic fields on living tissues is very complicated and at the moment insufficiently studied. Notwithstanding the considerable contribution which investigations of G. Ling [2], E. Del Giudice [3], A. Konovalov [4], E. Burlakova [5] and many other scientists made in the problem of low doses effects there are still many questions in this area to be solved. The review of modern state of the problem is given in [6].

Besides that, national standards for parameters in physiotherapy devices are different in different countries. Hence to estimate the effectiveness of magnetotherapy in practice physicians rely on experimental and statistical data about the results of treatment, which depend on parameters choice, the number and time of medical sessions, and other conditions.

To get closer to understanding mechanisms of curative effects of low frequency magnetic fields one may start from a modeling such processes. To do it we should choose adequate physical and mathematical models that take into account the parameters of environment, devices, and boundary conditions. In applications different types of devices functioning in a definite physical environment are used. A natural method of investigations is to construct a sequence of models, beginning form a simple one and complicating it step by step. One may consider the mathematical model describing the distribution of a magnetic field generated by coils which are in various configurations. Such configurations are used in many devices of magnetotherapy, so this model is not only a simple theoretical one, but it corresponds to real practical problems as well. The visualization of magnetic field intensity in the space may help a physician to match the obtained images and the results of application of curative sessions.

To better analyze the processes of action of low frequency magnetic fields one can complicate the first model and consider the model of ion movement in the field generated by a set of devices. In the first approximation we abstract physical environment structure and model the motion of an ion without regard interactions between ions. As in the first model, the visualization of phase portraits of the dynamical system describing this motion results in obtaining a set of images which presents typical structures for each selected configuration of parameters.

The action of the field may be studied both in air and fluid environment. Medical practice shows that the using mineral water leads to considerable improvement of the state for patients with diabetic neuropathy. So, to make next step in the complication of our model we have to consider ions motion in an environment and take into account possible interactions between ions and parameters of environment. At this step we probably will have to select essentially another model, which is not a complication of the previous one. When working in the air, the models applied in the dynamics of gas may be useful. As for the movement of ions in water (both in usual and mineral), the complexity of our problem increases considerably. Up to now there is no adequate model to study this problem.

Following this line of investigation we study a set of models, describing the processes in an environment, where a biological object is under the influence of electromagnetic field. It should be emphasized that these models characterize only external (in relation to the object) state of the environment and cannot be directly applied to the description of the internal state of the object. It is no doubt that there is a correlation between the processes in external environment and the changes which they cause in an organism. But it is unlikely that this correlation may be formulated in terms of mathematical dependences.

Nevertheless, in everyday practice of magnetotherapy one may estimate the curative effect indirectly by monitoring a patient health before and after sessions. These observations should be collected into a common set, database for example. The visualization of movement of charged particles makes the processes in the external environment more clear and gives a set of phase portraits generated by the mathematical model, which demonstrate typical trajectories for given parameters of a magnetotherapy device. Visualization helps a physician to form an associative set of images and to match it with statistical data of the results of a treatment.

In this work we propose the program system designed and implemented by us for modeling motion of an ion in electromagnetic field. The mathematical model is based on the of Newton second law, where the Lorentz force acts on the ion. By changing the initial data (device and ion parameters, coil parameters, etc.) we obtain visual representation of the ion trajectory. Actually the program serves as the example of imitational modeling and gives a possibility to obtain wide spectrum of phase portraits of the model system.

The paper is organized by the following way. In the next section we describe the method for approximate calculation of low frequency magnetic field, generated by a coil, in the points of a space grid. We also give the mathematical model for calculation of an ion trajectory in electromagnetic field. Section 3 contains the results of experiments for several configurations of fields: the motion in magnetic field, for common actions of electrical field and the field of the coil, and for the case when the both fields are periodic. In conclusion, prospects for further research by applying other models and the possibilities of practical application of the described program are discussed.

II. MATHEMATICAL MODEL AND METHOD OF SOLUTION

A. *Calculation of the magnetic field generated by a coil*

The calculation of magnetic field generated by a coil is well-known problem, which is solved when modeling magnetic field for several coils disposed arbitrary in a space. This problem arises in magnetotherapy devices. When calculating the field Maxwell's equations are used, and for low frequency field is assumed that electrical field generated by the magnetic field is negligible small. This assumption allows us to obtain analytical expressions (elliptic integrals of the first and the second kind) for components of magnetic induction vector. Usually these calculations are performed in cylindrical coordinate system of the coil, hence when dealing with arbitrary configuration of the coils one use additional local and global Cartesian coordinate systems. Elliptic integrals (components of magnetic induction vector) are calculated approximately in the points of space lattice constructed with a given step. Thus we obtain magnetic field of a coil as a tabular function on the lattice, and to calculate it in an arbitrary point we have to perform interpolation.

The problem of modeling magnetic field for an arbitrary configuration of coils was solved in [7], where all the used coordinate systems and transformation matrices were described. In [8-9] various variants of interpolation, optimization and visualization of calculations were considered. The results of modeling were applied to calculate and visualize the magnetic field intensity in a special magnetotherapy device. To visualize results the authors used ParaView package [10].

In this work the calculation of magnetic field of a given coil is a part of the problem about the modeling ion movement in electromagnetic field. The method of calculation follows the technic described above.

B. *Calculation of ion trajectory*

The detailed derivation of equations for the movement of charged particle in electrical and magnetic fields is given in many textbooks, for example in [11]. We describe them briefly. Consider a charged particle with a charge q and mass m. Let $\vec{E}(x,y,z,t)$ be the intensity of electrical field in the point (x,y,z) at the moment t, and $\vec{B}(x,y,z,t)$ be the magnetic field induction. The force acting the ion in electrical field is equal to $q\vec{E}$, and the Lorentz force in magnetic field equals $q\vec{v}\times\vec{B}$. The equation for ion motion has the vector form $m\frac{d\vec{v}}{dt} = q(\vec{E} + \vec{v}\times\vec{B})$. Assuming that $\vec{B}$ is co-directed with Oz, and hence $B_z = B, B_x = B_y = 0$, we obtain the following system of equations

$$\begin{cases} m\ddot{x} = q\big(E(x,y,z,t)\sin\gamma\cos\beta + \dot{y}\,B(x,y,z,t)\big) \\ m\ddot{y} = q(E(x,y,z,t)\sin\gamma\sin\beta - \dot{x}B(x,y,z,t)) \\ m\ddot{z} = qE(x,y,z,t)\cos\gamma. \end{cases} \quad (1)$$

Positions of vectors $\vec{B}$ and $\vec{E}$ are shown on Fig.1.

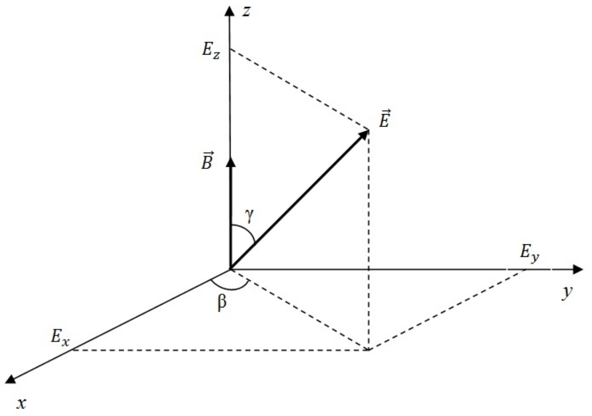

Fig. 1. The mutual disposition of vectors of electrical intensity $\vec{E}$ and magnetic induction $\vec{B}$.

The system (1) has analytical solution when uniform We solve the system by using the second order difference system. Denote by $[t_0, T]$ the time interval on which a trajectory is calculated, $t_i = t_0 + ih, i = 0, \dots n, x(t_i) = x_i, y(t_i) = y_i$, $z(t_i) = z_i$. For approximate calculation of first and second derivatives we use the following formulas

$$\ddot{x} \approx \frac{x_{i+1} - 2x_i + x_{i-1}}{h^2}, \ddot{y} \approx \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2}, \ddot{z} \approx \frac{z_{i+1} - 2z_i + z_{i-1}}{h^2}, \quad (2)$$

and

$$\dot{x} \approx \frac{x_{i+1} - x_{i-1}}{2h}, \dot{y} \approx \frac{y_{i+1} - y_{i-1}}{2h}, \dot{z} \approx \frac{z_{i+1} - z_{i-1}}{2h}. \quad (3)$$

Substituting (2) and (3) in system (1) we obtain the following second order system of difference equations

$$\begin{cases} x_{i+1} - K_i y_{i+1} = 2x_i - x_{i-1} - K_i y_{i-1} + L_i \sin\gamma \cos\beta \\ K_i x_{i+1} + y_{i+1} = 2y_i - y_{i-1} + K_i x_{i-1} + L_i \sin\gamma \sin\beta \\ z_{i+1} = 2z_i - z_{i-1} + L_i \cos\gamma, \end{cases} \quad (4)$$

where $K_i = \frac{qh}{2m} B(x_i, y_i, z_i)$ if current is constant, and $K_i = \frac{qh}{2m} B \cos \omega t_i$ in the case of variable current with frequency ω. By analogy $L_i = \frac{qh^2}{m} E(x_i, y_i, z_i)$, if electrical field depends on the point, and $L_i = \frac{qh^2}{m} E \cos \omega t_i$ for periodic field. The system (4) is linear, coordinates of z are found independently from x and y, and on every step x_{i+1}, y_{i+1} are calculated by Cramer method as $\Delta = 1 + K_i^2 \neq 0$.

Thus, depending on chosen configuration the system of difference equations is modified. In the case if only magnetic field of a coil acts, we at first calculate it by the algorithm described above and then construct a trajectory of an ion with given initial data in this field.

We should refine the algorithm for calculation of an ion trajectory to explain the connection between used coordinate systems. Let points $P_{i-1} = (x_{i-1}, y_{i-1}, z_{i-1})$ and $P_i = (x_i, y_i, z_i)$ of a trajectory be known in global coordinate system. To obtain the next point P_{i+1} we have to calculate $B(x_i, y_i, z_i)$ (taking this value from the table or performing an interpolation), take the local coordinate system in P_i and calculate in it coordinates of P_i, P_{i-1}. Then using equations (3) we obtain coordinates of P_{i+1} in local system and transform them into global system. Similar transformations are made when calculating $E(x_i, y_i, z_i)$. Hence, on every step our discrete system is solved in a local Cartesian coordinate system which depends on the position of the point P_i. It follows that angles β and γ in the right sides of equations (4) change from point to point. By virtue of the fact that the expressions $E \sin\gamma \cos\beta = E_x$, $E \sin\gamma \sin\beta = E_y$ and $E \cos\gamma = E_z$ are projections of E on coordinate axis they are calculated in the program by using built-in mathematical functions.

III. RESULTS OF EXPERIMENTS

Using the elaborated computer program we investigated various cases of action of electric and magnetic fields. In all examples shown below we assume that external parameters are the following:

- the size of the region (in mm) is $600 \times 300 \times 500$;
- the size of a cell of the lattice (in mm) is $4 \times 4 \times 4$;
- coil parameters are: center position is $(0, 150, 250)$, vector of axis is $(1, 0, 0)$, external radius is 58 mm, height is 34 mm, current intensity is 3A, the number of turns is 20, the number of windings is 25;
- h (in sec) is 10^{-6}.

Example 1. Calculate the trajectory of ion with $m = 96u$ (atomic mass units), $q = -2 * 10^{-19}$C, with initial points $P_0 = (x_0, y_0, z_0) = (100,150,200)$ and $P_1 = (x_1, y_1, z_1) = (100, 150, 200.01)$ in the magnetic field of a coil. Results of calculation are shown below on Fig.2.

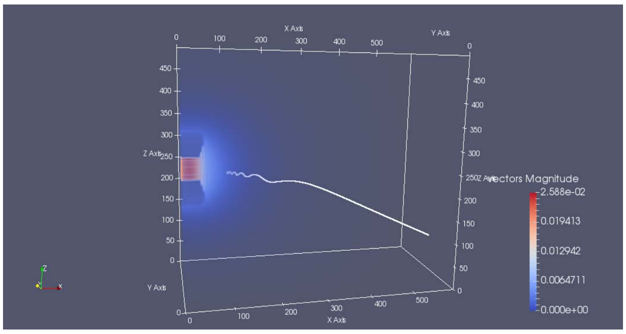

Fig. 2. The trajectory of ion in magnetic field of a coil for data given in Example 1.

Example 2. Consider Example 1 with other initial data.

Let $P_0 = (100,100,200)$, $P_1(99.99,150,200)$. The result is shown on Fig.3. We see that the motion depends on initial data considerably.

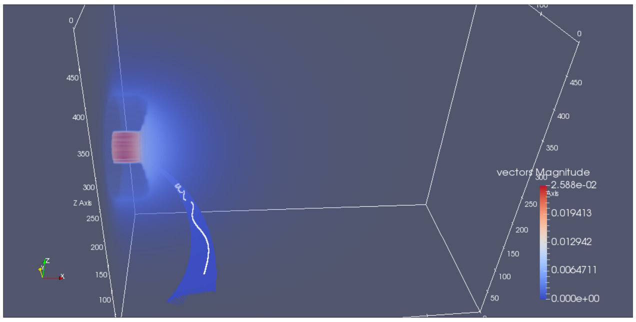

Fig. 3. The dependence of the ion trajectory in magnetic field on initial data.

Example 3. Now consider the motion of this ion when both magnetic and electrical fields act. Electrical field vector $E(0.01, 0, 0)$, $P_0 = P_1 = (300,150,210)$. The result is illustrated on Fig.4.

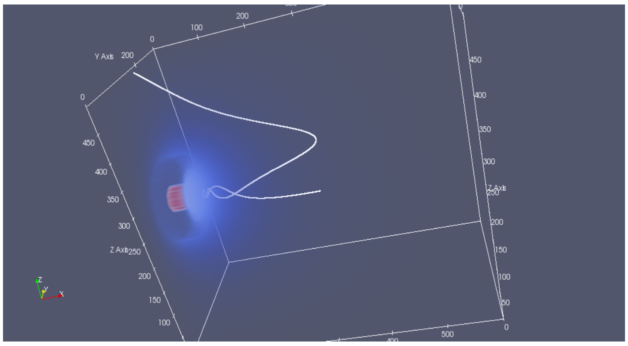

Fig. 4. The movement of ion in the case magnetic and weak electrical fields action.

Example 4. Take the same initial points as in Example 3, but change electrical intensity vector: $E(0.1,0,0)$. Now the trajectory has more simple motion, as Fig.5 shows.

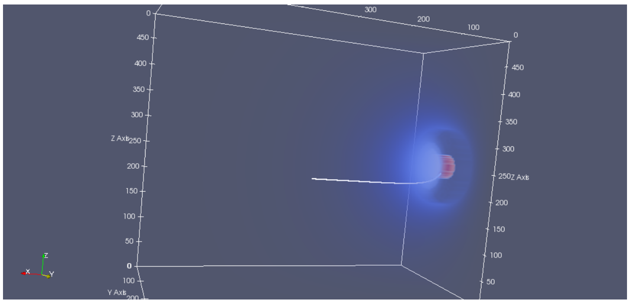

Fig. 5. The trajectory of ion motion when the electrical field intensity dominates.

Example 5. Now we consider the motion of ion when periodic electrical and magnetic fields act. Both fields have frequency 20Hz. The trajectory with initial data $P_0 = P_1 = (300,130,210)$ is shown on Fig.6.

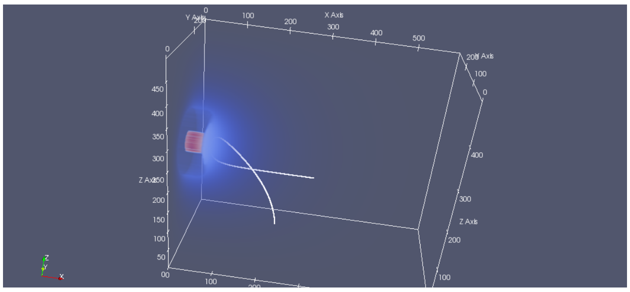

Fig. 6. The trajectory of ion when magnetic and electrical fields are periodical with the same period.

IV. CONCLUSION

Both physio- and magnetotherapy devices, where low frequency and low intensity magnetic and electrical fields are used, are widely applied in medicine. Curative actions of such fields are estimated mainly basing on practical results. In actual fact, the effects of influence both weak fields and low doses of medicine on living organisms is very complicated task. During several last decades many scientists are deeply involved in its solving. This problem calls for coordinated investigation from physics, biophysics, biologists, and chemists. One of approaches to understanding complex influence of magnetic field on living organisms lies in using statistical data about the patient state before and after treatment. For better interpretation of the obtained results, the processes in the external (in relation to the living object) environment must be taken into account. With this in mind we propose to use a sequence of gradually complicated mathematical models which describe the distribution of magnetic and electrical field intensities and the movement of charged particles (ions) in the environment. The implemented by us program may serve as an example of imitational modeling and is suitable to calculate the trajectory of an ion for the given configuration of the fields. Changing the parameters of the used device and visualization of results give a researcher the possibility to form a set of images which are typical phase portraits of the model system. For further investigations to study the motion of ions in air or water other models are required. And this subject is our future purpose.

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