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MODELING OF FERRIC NANOPARTICLES Fe^{3+} INTERACTIONS WITH THIN FILMS OF ORGANIC SUBSTANCES

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Abstract**—***The results of solving the problem of modeling the interaction of iron Fe^{3+} nanoparticles with thin bilayer membranes were represented. The purpose of the work was to create a physical model of the behavior and interaction of Fe^{3+} iron nanoparticles, which are located near thin films of organic substances. For this, physical model systems with thin films - BPM (bilayer phospholipid membranes) and BLM (bilayer lipid membranes) were considered and analyzed, and iron nanoparticles were introduced into these systems. To fulfill the given task, the data search methods ("data mining") obtained by the gas-liquid chromatography were used, as well as ones obtained in experiments with registration of transmembrane electric currents through artificial two-layer BPM and BLM membranes, and partially ones from the experiments on natural membranes with technique of voltage clamp. Since the applied $FeCl_3$ undergoes hydrolysis, the formed hydroxyl groups interact with BLM membranes, also participating in the sum of interaction effects. Thus, it was concluded about the important role of hydroxyl groups in the mechanism of anionic selectivity of BLM, which is a confirmation of previously obtained research data. A number of effects with participation of ionophores, which increase the ion permeability of artificial BLM membranes, were also considered; they can bind metal ions due to ion-dipole interaction. The described system with a membrane and iron (III) ions located near it can be used to study a number of phenomena on both artificial and natural membranes, for example, when iron nanoparticles were absorbed by human body from the environment. For all considered cases, known physical and physico-chemical regularities and the corresponding developed mathematical apparatus were verified. Namely, analytical expressions based on electrostatic interactions of electric charges associated with Fe^{3+} ions and localized on membrane surfaces were valid for describing the considered effects. The considered model membranes are on the border between living and non-living nature. At the same time, these systems are simple systems to which the laws of physics and physical chemistry are applicable. And, in some cases, when developing some technical hybrid systems, they can play the role of biosensors. Due to their simplicity, such models can be reproduced quite easily in the conditions of experiments, substances testing with analytical purpose in extreme situations. Therefore, such simple, reliable, tested methods can be used in wartime situations with limited laboratory resources.*

Index Terms—Modeling; physical model; Fe^{3+}; ferric ions; biosensor; bilayer membranes.

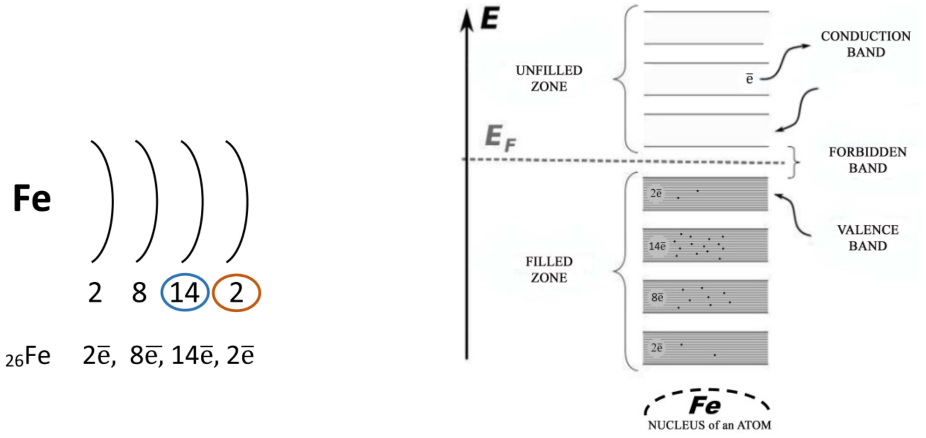
I. INTRODUCTION

Nanoparticles containing iron (Fe) follow each person from birth to the last minutes of life. The role of iron as element, its various oxides and other compounds is extremely large both in the economy (including in aircraft construction, aviation and space industries in general), as well as in technologies and scientific researches. In recent years, scientific researches in the field of ecological pollution prevention and its liquidation were intensified, including pollution with metal compounds (iron, lead, mercury, aluminum, chromium, others). It has happened due to the entry of these elements into the natural environment because of technogenic reasons: human economic and military activity, emergency situations and disasters, etc. [1] – [8]. The interests in the properties of iron nanoparticles is increasing now, in Ukraine because of the war reasons – the level of contamination of the natural environment of our country with compounds of various metals is increasing every day [2] – [4]. From other side, interest to the mechanisms of different nanoparticles interaction with organisms inner media increasing from day to day [9] – [18], and present work can clarify some of such mechanisms for ferric nanoparticles – ones, which concentration in our nature increasing due to the current military activities.

II. PROBLEM STATEMENT

It is known that various iron compounds are included into biomolecules of living organisms [2], [8]. Therefore, entering organisms as part of environmental pollutants, they can cause an imbalance in the biochemical reactions of bioorganisms, cause a number of disorders – so the relevance of further research of these problems is extremely high. Researching the outlined problem situations, the attention of scientists is attracted by a certain parallelism, the similarity of certain phenomena and processes involving iron nanoparticles, which have been registered by scientists in living and non-living nature. From the point of view of theory, this does not seem surprising, since in both cases the basis lies in the physical and chemical properties of iron as chemical element (Fig. 1). Indeed, it is surprising that studying the effects of iron atoms and ions in living nature, scientists sometimes have to appeal to the results of the works of scientists working with materials in engineering – so, to works in sufficiently distant field [19], [20]. At the National Aviation University in Kyiv, Ukraine, intensive experience has been obtained over the decades in several related areas: metal processing technologies [19], [20], environmental protection from industrial pollutants (including metal pollution in aviation, cosmonautics, ground services in airports, etc.) [1] – [7]. The authors of this publication have been working for many years to solve problems related to the outlined ones. This is the creation of information systems for monitoring of various harmful chemicals in the environment [21] – [25], development of software models [22], [25], mathematical models [26], and mathematical methods in general for solving linked problems [27] – [29].

The *purpose* of this publication was the creation of physical model of iron F^{3+} properties and behavior in interaction with films of organic substances. So, such models has to reflect some real effects of F^{3+} consumption from environment and their consequences for organism at cellular membrane level. Considering the heavy contamination of the environment by metals and their compounds in Ukraine, currently caused by the war and the need to take special measures in this regard [2], [3], the importance of work in this direction is really high.



a)

b)

Fig. 1. The most general contemporary imaginations about an atom of iron:
(a) is the scheme of electronic levels of the atom of iron (“planetary model”). The ovals indicate: blue – a cluster of electrons on the penultimate level (third layer from the nucleus), red – valence electrons on the outer level;
(b) is the energy levels of the iron atom. Schematic representation (details see in text)

III. PROBLEM SOLUTION

A. Methods

Creation of physical models was done basing on the series of results. Data mining in fields of ferric contamination of the ground and water was based on the results of the gas-liquid chromatography. In some experiments the comparison with effects at living cells were done; so, the technique of voltage clamp was used (Figs 2, 3). For conductivity characteristics analysis the registration scheme with the membrane, placed on the round pore was used (Fig. 2) with further development of this method – experiments with registration of transmembrane electric currents through artificial bilayer phospholipid membranes (BPM). Thin BPM films were studied under the conditions when aqueous solutions of electrolytes were washed on both sides of the BPM (an analogue of the state of the surface membranes of biocells), and on both sides of such membranes electrodes were included in electric circuit with placed current meters. It must be remembered that in the conditions of war it is necessary to give preference to analytical methods that are the most simple to perform, reliable and repeatedly used. In such a way it was possible to register transmembrane electric currents, changes in the characteristics of which indicate changes in the states of the systems and the emergence of the so-called anion selectivity, in which hydroxyl groups play important role [8].

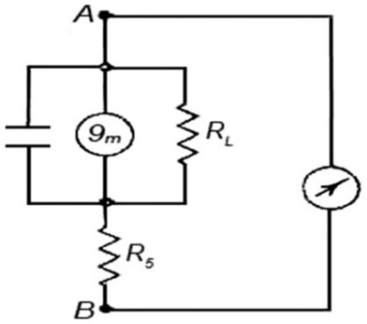


Fig. 2. Equivalent scheme of the experiment with bilayer phospholipid membranes [8]: R_L is the leakage resistance; *Rs* is the series resistance (determined mainly by the resistance of the pore for dialysis; transmembrane potential difference is measured (and clamped) between points *A* and *B*)

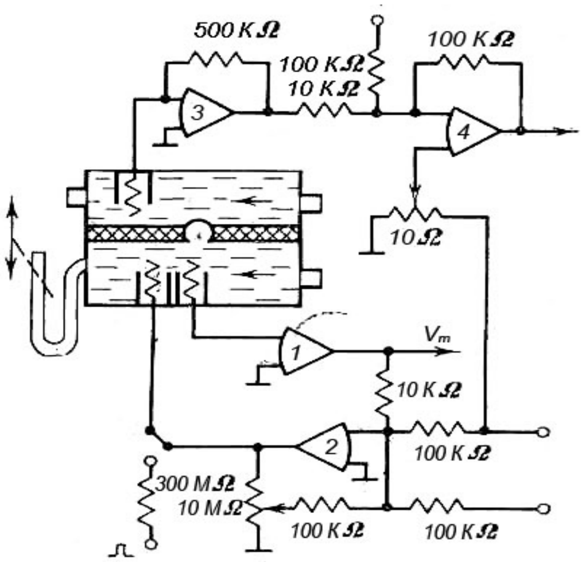


Fig. 3. Scheme of the experimental setup which can be used for the dialysis of a) artificial membrane, or b) natural membrane of a cell {f.e.neuron) in voltage clamp conditions (one of biosensor prototypes) [8]. General configuration of the method: 1 – input amplifier; 2 – voltage clamp amplifier with adjustable amplification; 3 – current amplifier; 4 – intermediate amplifier for communication with external devices and compensation of leakage current, pressure adjustment is indicated by a vertical arrow. Pore for dialysis in horizontal plate that divides the experimental container into 2 compartments; solutions in each compartment can be changed

B. Model systems

If we are speaking about the environments in which the contact of iron atoms and ions (see Fig. 1) with biomolecules most often occurs, then these are often thin films of organic compounds. In general, the problems of the interaction of iron ions of different valence, including Fe^{3+} ions, with thin and thick films of different compositions have been studied for a long time [8]. The wide variety of obtained experimental results does not allow us to outline a comprehensive picture of the registered phenomena united by a single theory. Below we will consider the results of experiments on artificial bilayer phospholipid membrane (BPM), which in experimental conditions can form the thin bilayer membranes (BLM membranes). Bilayer phospholipid membrane can be considered as a model of protoplasmic cell membrane as well, the surface of lung cells or the cells of gastrointestinal tract, some others, through which $FeCl_3$ environmental pollutants can enter the human organism and cause a number of phenomena (including negative ones) [2], [8], [30]. So, let's consider physical model systems with thin films – BPM (BLM in general), into which iron nanoparticles were introduced.

C. Models of some effects with ferric ions

Bilayer lipid membranes are widely used as models for studying the interaction of ions with organism membranes, etc. Their resistances are in interval 10^8 – 10^9 Ohm· cm^3. Such systems can act as models of membranes on the surface of living cells in the lungs, gastrointestinal tract of a person or animal, which were exposed to iron nanoparticles when inhaled or licked in a polluted environment. Since such membranes are poorly permeable to hydrophilic substances and almost impermeable to ions, substances have been found that increase the ionic permeability of artificial BLM membranes. For this purpose, ion carrier substances (ionophores) are used, which bind metal ions through ion-dipole interaction with the polar groups that make up their molecules. This type of ion binding is sometimes called intramolecular dissolution.

Hydroxyl groups that appear in the result of $FeCl_3$ hydrolysis play their important role of in the processes of interaction of ferric ions with model membranes, in the mechanism of anion selectivity of BPM. These conclusions were supported by the research data [2], [8], [31]. In numerous experiments there were registered that when small amounts of $FeCl_3$ (final concentration 10^{-6}–10^{-4} M) were introduced into a NaCl solution having a pH of 4–6.5, the resistance of the BPM decreases by 5–6 orders of magnitude and an almost ideal anionic electrode function was established. As it known, in this pH region, $FeCl_3$ undergoes hydrolysis with the formation of products such as $Fe(OH)_3$, $FeOH^{2+}$ and $Fe(OH)_2^+$ [31]. When $FeCl_3$ is introduced into solutions whose pH is below 4, changes in the conductivity and selectivity of BPM occur only when agents that promote the hydrolysis of $FeCl_3$ are simultaneously introduced into this solution. At the same time, the introduction of a suspension of iron hydroxide into a solution does not in itself lead to changes in the properties of the bimolecular layer. Based on this, it was concluded that changes in the conductivity of BPM arise as a result of series of reactions, including first the interaction of polar groups of lipids with ferric ions and the subsequent formation of iron hydroxides already included in the membrane structure. The relatively slow establishment of the final resistance values of the latter confirms or, in any case, does not contradict such a hypothesis. The special role of iron hydroxides in the emergence of anion conduction channels in BPM was proven by a number of experiments [31]. These include experiments that have shown that the introduction of a reducing agent (hyposulfite) into solutions completely removes the effect of increasing the conductivity of the membrane, the resistance of which increases to its original values. The fact that the effect of $FeCl_3$ is also detected when solutions of dipalmitoylecithin, i.e., a lipid with fully saturated fatty acid residues, are used to obtain BPM, allows us to exclude the role of autoxidation of unsaturated fatty acid chains present in lecithin of natural origin, stimulated by Fe^{3+} ions. Special electrophoretic and spectral studies carried out on lecithin dispersions showed that the lipid binds mainly non-hydrolyzed or incompletely hydrolyzed iron salts, and hydrolysis in the presence of lecithin proceeds more slowly than in conventional aqueous solutions of $FeCl_3$. The latter, probably, reflects changes in the reactivity of iron ions when they interact with charged lipid groups.

For membranes in NaCl solutions (in the presence of $FeCl_3$), the anion transfer numbers found from the slopes of the concentration dependence curves turned out to be equal or close to unity [31]. Determinations of ^{36}C1- fluxes through such membranes at different values of the current flowing through them showed good agreement with the calculated values of C1- fluxes obtained under the assumption that the current transfer by cations under these conditions is negligible ($t_+ = 0$). Unfortunately, in this interesting work there were no determinations of membrane specificity in the series of monovalent anions or at least a qualitative comparison of the permeabilities of singly and doubly charged anions. Meanwhile, this would make it possible to clarify the role of the sizes of anions and the magnitude of their charge in the permeability of the membrane for them.

The changes in the conductivity of BPM caused by the introduction of $FeC1_3$ into solutions turned out to depend on the concentration of sodium chloride. When the concentration of NaCl was reduced to 10^{-3} M, the introduction of $FeCl_3$ into solutions was no longer effective. On the other hand, a nonlinear dependence of the conductivity of BPM on the concentration of $FeCl_3$ introduced into solutions was discovered. In general, this dependence had the form of S-shaped curve, and there were no changes in conductivity at $FeCl_3$ concentrations less than 10^{-7} M, and were insignificant at concentrations above $2 \cdot 10^{-5}$ M.

The current-voltage dependences of the BPMs modified by the introduction of ferric iron showed a clearly defined superlinearity and did not differ in appearance from the corresponding curves obtained when studying membranes modified by the introduction of valinomycin and having the opposite electrode function. In the region of potential differences on the membrane exceeding 60 mV, the current-voltage characteristics in both cases are satisfactorily described by the Tafel equation

$$\varphi = \alpha + \beta \ln \boldsymbol{I},$$

where α, β are constants; φ potential difference; $\boldsymbol{I}$ electric current.

The anion selectivity of BPM modified by introducing $FeCl_3$ into solutions can be changed to a fairly pronounced predominant cation permeability in solutions with NaCl $t_+ = 0.82$. This occurs when chemical agents are introduced into the solutions separated by the membrane; f.e. agents that form complexes with iron ions (citrates, oxalates, thiocyanates, EDTA). It is very noteworthy that the transition from a pronounced anionic to a predominant cationic electrode function may not be accompanied by a change in membrane resistance, but a change in the electrode function requires a certain time (1–1.5 min) and a 10–30-fold excess of the complexing agent relative to the initial amount of $FeCl_3$. In article [31], the specificity and selectivity series for alkali metal cations were not determined, and the nature of the current-voltage dependences for membranes that acquired a cationic electrode function was not established. The latter would make it possible to establish the similarity or difference between the phenomenon of change in electrode function found here and that observed in cases of BPM modified by the introduction of antibiotic alamethicin when protamine was added to solutions. As mentioned, despite the reversal of the cation-anion selectivity of the BPM, the character of the current-voltage curves was the same/ This made it possible to think about the difference in the structures responsible for the sensitivity of the conduction channel to the magnitude of the electric field on the membrane and its ion selectivity.

Not only the high anion selectivity of BPM modified by the introduction of $FeC1_3$, but also the possibility of obtaining membranes with pronounced asymmetric electrochemical properties (rectification in systems asymmetric with respect to $FeC1_3$), as well as the clearly expressed phenomenon of delayed rectification, make these membranes a valuable model of protoplasmic cell membranes. Therefore, the interest in elucidating the nature of ion selectivity and the mechanisms of anion transfer in such systems is understandable.

Since when $FeC1_3$ is introduced into a solution on only one side of the membrane, the asymmetry of the latter is maintained for a long time, it is obvious that the rates of transition of Fe^{3+} ions and iron hydroxides through the membrane are quite low [31]. Taking into account also the data of direct measurements of $^{36}C1$- fluxes when passing current through membranes, we have to consider the hypothesis about the existence in these cases of positively charged mobile carriers in the membrane (for example, Fe3+ ions or positively charged iron hydroxides) unacceptable. The assumption of the presence of a neutral form of the carrier, as which would be the neutral form of iron hydroxide, can be consistent with the data on the fluxes of $^{36}C1$-. However, in this case, the reason for the affinity of such a carrier for anions remains unclear. The existing observations are more consistent with the idea that a sharp increase in the conductivity of BPM when $FeC1_3$ is introduced into solutions is due the occurrence of packing defects in the fatty acid chains of phospholipids during the formation of iron hydroxides, previously bound by the phosphate groups of lipids, or the formation of hydroxide precipitates in the area where the polar groups of the bimolecular layer are located. In this case, disorganization in the hydrophobic zone of the BPM is induced by changes in the position of the polar groups. At the same time, it is easy to imagine that the channel penetrating the hydrophobic zone of the membrane does not have pronounced ion selectivity and the latter is set by boundary conditions, i.e., determined by the properties of chemical groups located at the entrance to the channel or even at some distance from it. This model makes it possible to explain the reversal of the cation-anion selectivity of membranes modified by the introduction of $FeC1_3$ in the absence of changes in their conductivity.

The packing defects of their fatty acid residues, which determine the conductivity of the bimolecular layer of phospholipids, should apparently be of a local nature [31]. This is indicated by the data on the binding of iron ions or its positively charged hydroxides by lecithin dispersions, from which it follows that only thousandths (or less) of the total number of phospholipid molecules are involved in such interactions. In addition, measurements that showed the constancy of the BPM capacitance values when introducing $FeC1_3$ into solutions should be considered as indication of the constancy of the average thickness and average dielectric constant of the hydrophobic zone of the bimolecular layer. The latter can be reconciled with the observed increase in membrane conductivity by 5–6 orders of magnitude only by assuming that violations of the initially existing packing of fatty acid chains occur in an area constituting a very small fraction of the total area of the membrane. Since the magnitude of this fraction remains unknown, it is impossible to draw conclusions regarding the electrical conductivity in the zones corresponding to such channels. Nevertheless, the mechanisms of ion transport in them must differ significantly from that observed for free electrolyte solutions, since, with a constant total channel area, only in this case can some explanation be found for the exponential dependence of conductivity on the potential difference on the membrane. An alternative explanation may be, however, the dependence of the number of such channels on the magnitude of the electric field.

IV. CONCLUSIONS

The author experience of implementation of 3G, 4G connections technologies at the territory of in present article the results of modeling of ferric Fe^{3+} nanoparticles interaction with thin bilayer membranes were described. All known regularities that were registered for such interaction and have analytical expressions, which were based on electrostatic interactions of electrical charges both on Fe^{3+}ions and the surfaces of such membranes are applicable for these cases. Above described system with the membrane and ferric ions located near it can be used to study a number of phenomena on artificial as well as natural membranes. The conclusion about the important role of hydroxyl groups in the mechanism of anion selectivity of BPM was supported by previously registered research data. Because $FeCl_3$ undergoes hydrolysis, these hydroxyl groups interact with BLM membranes, participating in the sum of effects of interaction too. Some effects of ionophores that increase the ionic permeability of artificial BLM membranes were observed; they can bind metal ions through ion-dipole interaction.

Because of their simplicity such models can be easily recreated in laboratory conditions. Such simple methods be used in wartime with limited laboratory resources and in extreme situations. Heavy contamination of the environment by metals and their compounds in Ukraine, currently caused by the war, and the need to take special measures in this regard increase the importance of present publication.

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О. М. Ключко, І. В. Морозова, М. Г. Ключко, І. В. Бурцева. Моделювання взаємодій наночастинок заліза Fe^{3+} з тонкими плівками органічних речовин

Розглянуто результати вирішення задачі моделювання взаємодії наночастинок заліза Fe^{3+} з тонкими бішаровими мембранами. Метою роботи було створення фізичної моделі поведінки та взаємодії наночастинок заліза Fe^{3+}, які знаходяться поблизу тонких плівок органічних речовин. Для цього було розглянуто та проаналізовано фізичні модельні системи з тонкими плівками – БФМ (біслойними фосфоліпідними мембранами) та БЛМ (бішаровими фосфоліпідними мембранами), в ці системи було введено наночастинки заліза. Для виконання поставленої задачі були застосовані методи пошуку даних («дата майнінг»), отриманих методом газорідинної хроматографії, у експериментах з реєстрації трансмембранних електричних струмів через штучні двошарові БФМ та БЛМ мембрани, частково також у експериментах на природних мембранах за методикою фіксації потенціалу. Оскільки застосована сполука $FeCl_3$ піддається гідролізу, утворені гідроксильні групи взаємодіють з мембранами БЛМ, також беручи участь у сумі ефектів взаємодії. Таким чином, було зроблено висновок про важливу роль гідроксильних груп у механізмі аніонної селективності БЛМ, що є підтвердженням отриманих раніше даних досліджень. Були розглянуті також ряд ефектів за участі іонофорів, що підвищують іонну проникність штучних БЛМ мембран; вони можуть зв'язувати іони металів внаслідок іон-дипольної взаємодії. Описана система з мембраною і розташованими біля неї іонами заліза (III) може бути використана для вивчення ряду явищ як на штучних, так і на природних мембранах, наприклад, при поглинанні наночасток заліза організмом людини з довкілля. Для всіх розглянутих випадків справджуються відомі фізичні та фізико-хімічні закономірності та відповідний розроблений математичний апарат. А саме, для описання розглянутих ефектів є справедливими є аналітичні вирази, які базувалися на електростатичних взаємодіях електричних зарядів, що пов’язані як з іонами Fe^{3+} , так і локалізовані на поверхнях мембран. Розглянуті модельні мембрани знаходяться на межі живої і неживої природи. У той же час ці системи є простими системами, до яких застосовні закони фізики та фізичної хімії, і в деяких випадках при розробці ряду технічних гібридних систем вони можуть грати роль біосенсорів. Завдяки своїй простоті такі моделі можна достатньо легко відтворити в умовах експериментів, тестувань речовин з аналітичною метою у екстремальних ситуаціях. Тому такі прості, надійні, апробовані методи можна використовувати у воєнний час у ситуаціях з обмеженими лабораторними ресурсами.

Ключові слова: моделювання; фізична модель; Fe^{3+}; іони заліза; біосенсор; двошарові мембрани.

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