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PHYSICAL AND MATHEMATICAL MODELS OF TWO TYPES OF BIOSENSORS

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***Abstract*—*In previous investigations the idea of development of two types of neuro-like biosensors - detectors of chemical substances in environment were grounded. In present article we have developed this idea deeply and substantiated the differences between two types of biosensors: biosensors and detectors with elements - artificially elaborated selective membranes. In this paper we described briefly both types of detectors as well. Further some their similar characteristics as well as mathematical description of physical phenomena at the surfaces of detectors was suggested. Such detectors were able to register hazardous chemical substances in the Nature. They included sensor elements covered with chemo-sensitive specific coatings – layers of organic and/or inorganic compounds. The purpose of present article was to demonstrate mathematical description of physical phenomena at the surface of biosensor that were similar to both types of detectors.*

Index Terms—Physical model; mathematical model; detector; sensor device; chemical substances.

I. INTRODUCTION

Research aimed at the creation and detailed study of membrane systems that model the basic physicochemical properties of protoplasmic membranes, including their ion selectivity, is becoming increasingly important. The latter is connected with the urgent need to create a theory of this most important mechanism. Living cells are characterized by the number of specific features: their microscopic size, instability of states and the exceptional complexity of the reactions of the cell as an integral system, limit the possibilities of detailed electrochemical studies and, especially, studies involving a wide variation of conditions (ionic strength, salt concentrations, pH, temperature, difference potentials on the membrane, etc.) This specificity has to be taken into account in processes of physical and mathematical modelling.

Even for solving relatively simple problems one has to face significant difficulties in studying the membranes of living cells; for example, for the registration of their current-voltage characteristics. In cases of founding of adequate models, these difficulties can be excluded. An important task of physical and mathematical modeling is to establish the physicochemical nature of the very phenomenon of ion selectivity of protoplasmic membranes and to resolve the question why the biological systems can be considered as exceptional or specific ones. Detectors we described now were able to detect chemical substances in the environment, both in the air and water phases. Invention and elaboration of such detectors were based on the theory of membrane systems. These detectors included sensor elements with chemo-sensitive specific layers like membranes or films. Being in contact with specific chemical substances, such detectors revealed the properties of chemo-sensitivity like real neuro-like systems. This is a reason why they were called sometimes “neuro-like biosensors”. Further we had subdivided neuro-like biosensors on to two groups [1], [2]. The first group includes technical devices with incorporated biological membrane, and the second group – devices and apparatus with inorganic coatings at their sensitive surface. Both types demonstrated phenomenon of chemo-sensitivity [1], [2].

The purpose of present article was to demonstrate mathematical description of physical phenomena at the surface of biosensor that were similar to both types of detectors.

II. PROBLEM STATEMENT

Detecting surfaces of neuro-like biosensors, being in contact with specific chemicals have to reveal chemo-sensitivity and; in some cases, even ability for primary processing of information [1], [2]. These characteristics of neuro-like biosensors were described in our previous works and the works of other authors [1] – [7]. In these works such biosensors further were incorporated into the information systems for the detecting of chemical substances in environment; in such a way chemical pollution of environment can be monitored [8] – [12]. In some cases such information systems included the expert subsystems; sometimes such unit can function separately as expert system [13] – [15]. Specific modern mathematical tools were used for such work [16] – [18]. Some mathematic models were developed in process of this work [18], as well as program models [19] – [21].

In process of all these works raised the necessity of mathematic description of physical processes at detecting surface – membrane, film, etc. It is possible to see that they demonstrated a lot of similarities in physics of scenarios for both types of neuro-biosensors. Below we suggest the mathematical description of such physical phenomena at the surface of detectors.

III. PROBLEM SOLUTION

Let's examine the case of ions presence above the surface of biosensor membrane. Being electrically charged particles, their behavior can be modeled using Coulomb's law and other physical laws of electrostatics. Internal energies of ions in the membrane can be represented as $\left(\bar{U}_i - \bar{U}_j\right)$:

$$\Delta F_{ij} = -RT \ln \bar{K}_{ij} = \left(U_i - U_j\right) - \left(\bar{U}_i - \bar{U}_j\right). \quad (1)$$

The first of the internal energy differences appearing in equation (1) can be found on the basis of tabular data. The difference between the internal energies of cations in an ion-exchange material, such as glass, can be approximately estimated if, in addition to the crystalline radius of the cation, some conditional value r^- is known, which is determined by the distance of the closest approach of the cation to the electric center of gravity of the anionic place in the glass. This value, which characterizes the strength of the anionic field of ion-exchange sites, according to the theory under consideration, determines the ion selectivity of the membrane.

The force of the Coulomb's interaction of two unit charges was:

$$f = \frac{e^2}{\left(r^+ + r^-\right)^2}, \quad (2)$$

where r^+ and r^- are the radii of approaching particles. The potential energy of two electric charges can be determined based on the amount of work when the distance changes by $d(r^+ + r^-)$ using the equation below. Since the work dA is equal to the loss of internal energy U, then

$$dU = \frac{e^2}{\left(r^+ + r^-\right)^2} d\left(r^+ + r^-\right), \quad (3)$$

or

$$U = \frac{-e^2}{r^+ + r^-} d. \quad (4)$$

If the charge values are expressed in electron charges, the distance between the centers of gravity of the charges is in angstroms, then the free energy of the Coulomb interaction of the cation (in vacuum), expressed in kcal-M^{-1}, is determined by the expression:

$$\Delta F_i \approx \Delta U_i = \frac{-332}{r^+ + r^-}. \quad (5)$$

To estimate the internal hydration energies of ions, Eisenman made a similar calculation of the interaction of a cation ($z = 1$) with the multipole of a single water molecule using the Rawlinson model. In this case, the free energy of ion hydration can be represented by the expression

$$\Delta F_i \approx \Delta U_i = -332\left(\frac{q_n}{r^+ + r_n} + \frac{q_p}{r^+ + r_p}\right), \quad (6)$$

where $q_n = -0{,}64e$ is the effective charge for the electronegativity center of the water molecule, and $q_p / 2 = +0.32e$ is the effective charge of each of the protons $\left(q_n = -q_p\right)$. The values $r^+ + r_n$ and $r^+ + r_p$ are the distances, respectively, from the center of electronegativity and from the centers of electro positivity of the water molecule to the center of the cation.

The similar scenarios were registered at the surfaces of glass electrodes. Very interesting feature of electrode glass membranes is that the current-voltage characteristics obtained under stationary conditions, are straight lines in a wide voltage range (in special experiments, the voltage was increased to 250 V). This linearity was not violated with a

pronounced asymmetry of the electrolyte composition of solutions, which nevertheless affects the transmembrane potential difference under zero current conditions. Thus, the glass electrode membrane shows no evidence of Goldman-type rectification, although for asymmetric electrolyte systems including a fixed-charge ion-exchange membrane, the nonlinearity of the current-voltage characteristic, according to theoretical considerations, should take place. In addition, for membranes with unknown thermodynamic properties, but having an ideal cationic function, to which electrode glasses can rightly be attributed, a general phenomenological equation for zero current conditions can be derived, which is identical to the Goldman–Hochkin–Katz equation

$$\varphi_{I=0} = -\frac{RT}{F}\ln\frac{\sum^{n} P_{i^+} C_{i^+}^{\text{in}} + \sum^{n} P_{i^-} C_{i^-}^{\text{out}}}{\sum^{n} P_{i^+} C_{i+}^{\text{out}} + \sum^{n} P_{i^-} C_{i^-}^{\text{in}}}, \qquad (7)$$

without a special assumption regarding the linearity of the electric potential profile in the membrane. If this is so, then the described case is in sharp contradiction with theoretical predictions, since from the experimental curves shows, that the equality is not satisfied:

$$\frac{a'_H}{a''_H} = \frac{\lim G_{\varphi\to-\infty}}{\lim G_{\varphi\to+\infty}}, \qquad (8)$$

where the limiting conductivities must correspond to the values of the slopes of both branches of the current-voltage characteristics. The reason for these differences, it seems, is associated with the carrier change process, which can be the limiting stage in current transfer and which was not taken into account in the above theoretical considerations. The independence of the resistance of membranes from cation-specific glasses from the composition of aqueous solutions suggests that in these cases the equality should not be satisfied:

$$\frac{1}{K_{ij}} = \frac{G_i}{G_j}, \qquad (9)$$

where G_i and G_j are the conductivities of the glass membrane, determined under symmetrical electrolyte conditions.

IV. CONCLUSIONS

Brief review of characteristics of neuro-like biosensors was done in present article. Such biosensors were sensitive to chemical substances, so, they can be used as detectors of molecules-pollutants in environment. Such biosensors can be subdivided to two main groups. The first group included detectors with functions very close to real biological objects, f.e. neurons; which were sensitive to chemical compounds and ions, like bio-objects (cellular membranes, others) [4], [5]. The second group of biosensors united detectors with artificial surfaces, covered with the layers with ion-selective characteristics. They could be produced artificially, like electrode ion-selective glasses [3]. The mathematical description of physical phenomena at the sensitive surface of neuro-like biosensor was represented. In the article the theoretical basis for the elaboration of neuro-like biosensors with chemo-sensitive surface was suggested.

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І. В. Морозова, О. О. Колганова, Д. А. Навроцький, І. В. Бурцева, А. М. Миколушко. Фізична та математична моделі двох типів біосенсорів

У попередніх дослідженнях була обґрунтована ідея розробки двох типів нейроподібних біосенсорів – детекторів хімічних речовин у навколишньому середовищі. У цій статті глибоко розвинено цю ідею та обґрунтовано відмінності між двома типами біосенсорів: біосенсорами та детекторами з елементами – штучно розробленими селективними мембранами. У статті також коротко описано обидва види детекторів. Далі було наведено деякі їх подібні характеристики, а також математичний опис фізичних явищ на поверхнях детекторів. Такі детектори могли реєструвати небезпечні хімічні речовини в природі. Вони містили сенсорні елементи, вкриті хемо-чутливими специфічними покриттями - шарами органічних та/або неорганічних сполук. Мета цієї статті полягала в тому, щоб продемонструвати математичний опис фізичних подій на поверхні біосенсора, які були подібними у детекторах обох типів.

Ключові слова: фізична модель; математична модель; детектор; сенсорний пристрій; хімічні речовини.

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