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INFORMATION TECHNOLOGIES: PHYSICAL AND MATHEMATICAL MODELS OF DETECTORS FOR ENVIRONMENT MONITORING SYSTEMS

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Abstract*—Ecological monitoring is a real need in contemporary world with its growing tendency of environmental industrial pollution. Among such pollutants there are chemicals emanated in fires, explosions and other emergencies, in process of ruining of chemical enterprises, enterprises of oil and gas cycle, and etc. Some information systems for appropriate monitoring were described briefly in this article together with incorporated hybrid system of electronic chemical pollution detectors that were able to input information to such systems. In previous works of the authors the necessity of development of two types of such detectors with specified properties were substantiated: biosensors and detectors with elements – artificially elaborated selective membranes. This article describes the second type of detectors. The proposed detectors were able to detect harmful chemicals in the environment in the air and water phases; development of such devices was based on the theory of membrane systems. The detectors contained sensor elements covered with chemo-sensitive specific coatings – layers of substances: membranes, films, etc. When in contact with certain chemicals, these detectors demonstrate the properties of chemo-sensitivity and primary identification of such compounds. These studies were aimed on developing detectors of various environmental pollutants based on the theory that can be used as a basis for the detection of such substances. The works were based on a deep study of membrane systems with further development of physical and mathematical models of some substances detection taking into account basic chemical and physical properties of artificial and natural membranes, as well as their ionic selectivity. Some results of mathematical modeling of such detectors with artificial membranes – chemo-sensitive surfaces – were described in the article. Summarizing the previous experience, a brief review of authors' publications in these items was done, as well as the works of some other authors. The purpose of the work was, basing on profound studying of artificial membrane systems, to suggest them as physical model and summarize the experience of development of their mathematical models.*

Index Terms—Information system; physical model; mathematical model; detector; sensor device; fires; chemical substances; chemical pollution of environment.

I. INTRODUCTION

Our contemporary reality is characterized by intensive industry development with subsequent chemical pollution of environment, cruel wars with explosions, fires, other emergencies with emanated chemicals, in process of ruining of chemical enterprises, as well as enterprises of oil and gas cycle, and etc. Chernobyl accident in Ukraine was a shock for the whole World, its consequences we felt to the current days, and it faced us with the necessity of practical protection of the environment. Such antropogenic and technogenic disasters usually happened with emanation of harmful and/or toxic chemicals, and the task of their detection in environment is important indeed to save the life and health of people, other biological organisms, finally, to save the Nature in whole [1] – [5]. Actually, the development of information systems with such chemo-detecting elements for data input, as technical devices (robots, drones, etc.) are necessary indeed. [1] – [4], [6] – [9]. Such detecting devices with functions of sensitivity for different chemical substances in environment can be used as elements

of large-scaling information system [10], [11]. Detecting subsystem for such devices can include sensory elements, like chemo-sensitive membranes (of natural origin and/or artificial ones), layers from specific substances, coatings, and etc. [10], [16]. Such elements being in contact with some acted chemicals have to reveal chemo-sensitivity and; in some cases, even ability for primary processing of information, doing initial identification of these substances [10], [11].

In our article the data about the information system (IS) with chemo-sensitive detectors of biosensor nature were presented. Theoretical bases for novel detectors elaboration for the IS were demonstrated, aimed on further their use for mathematical model development. The *purpose* of present work was to study potential detectors for the IS profoundly, to suggest their physical model and to summarize the experience of its mathematical models development.

II. Problem Statement

Developing the information system with incorporated elements for chemo-sensitivity is necessary, in the first order, to solve the problem of sensitive detectors of high quality as well as problem of the data input in general. Some prototypes of such ISs had been already presented in some our works as well as the works of other authors [1] – [4], [6] – [11], [16]. One of such automated information system (AIS) had been described in [1] – [4]. The structure of AIS can include several pulsed spray devices and AIS that control their work with a network of sensors for fixing flame and smoke, as well as thermal imager and video cameras (the system AIS ASCOP [1] – [3]). They show, record and analyze the reliability of data on the current parameters of the fire, and predict trends in its further development basing on data from the zone of surrounding fire. Other example is "EcoIS" system for monitoring of ecological state of environment, invented by Dr. Klyuchko OM [6] – [9]. The purpose of this work was the development of new informational system for environment monitoring in wide time ranges using modern information and computer technologies, on the base of novel electronic information systems with databases. During the work following methods were used: methods of comparative research of the samples of technical devices, imitation and program modeling, which were based on numerical results obtained in experiments with the recording of chemo-sensitive transmembrane electrical currents in neurons in voltage clamp mode and other methods. Used biophysical methods permitted to reveal and identify substances, hazardous for living organisms and to make the first conclusions about their possible biological influence. In result the original system has been developed for environment monitoring in broad time ranges (from the first moments of substances influence on single organism cells – to months and years after this influence on whole organism). This information system was coupled with detector groups, databases (DB), expert subsystem and interfaces. It was able to distinguish between certain types of chemicals at the input; to display their identification data and, if necessary, reports about their harmfulness [7], [9]. "EcoIS" system was suggested for the use in ecological scientific and academic practice, for environment protection. Detailed analysis and studying of peculiarities of biological objects and necessity to use of mathematic and other methods that was not used before become the basis for the DB development. The series of these works were continued by the elaboration of some other versions of "EcoIS" with DBs, including DB of images, electronic expert system and electronic working places for it, linked with DB for few specialties (ecologists, zoologists, etc) [6], [7], [9].

Input data for such ISs were obtained from the detectors incorporated into IS; they have to be sensitive to harmful chemical molecules in environment. Two main groups of detectors can be used for such purposes. The first one group included detectors developed on idea of biosensor [10] – [13], with "biosensor-like" functions, which were sensitive to chemicals like biological objects (cells, their membranes, etc.) [10], [11], [13]. The authors have already developed some versions of ISs with such "biosensor-like" detectors [10], [11]. Other, the second group of detectors included detectors with surfaces, covered with thin layers, films or membrane with ion-selective properties. They can be done in artificial manner, like ion-selective glasses of electrodes [14] – [16], and we studied theoretical possibility to incorporate them into developed IS [7], [10], [11], [17], [18]. The first works with such glasses were done previously by B. P. Nikol'sky and then by A. A. Lev [19], [20]. Such specific sensory elements (chemosensitive membranes (artificial and/or natural origin), specific coverings and layers of substances) after the contact with certain environmental chemicals are able to form the signals about pollutants presence and, in some cases, to perform their initial identification [14] – [16]. The latter is the most desirable for the development of multi-functional portable sensors. Studies aimed on the construction of devices for the detecting various

environmental pollutants were based on a detailed study of membrane systems that simulate the main physicochemical properties of artificial and natural membranes, including their selectivity to ions; and such studies were becoming increasingly important [14] – [16].

This is especially necessary during a fire extinguishing and eliminating of other consequences of accidents, catastrophes at large industrial enterprises and objects of energetic, when extinguishing algorithms have to be linked quickly with current state of the object. The automated system that control the processes of extinguishing and liquidation of emergency situation have to work in real time, limited by the specifics of the controlled process and corresponding to the transition of the fire or emergency situation into an uncontrolled fire or techno gene disaster [14] – [16]. In any modern enterprise it is very important to ensure quick, effective and reliable extinguishing with strictly metered commissioning of extinguishing means and thereby ensuring the lowest possible changes of technological regimes. The currently used automatic fire extinguishing systems based on traditional executive inertial devices and installations for supplying fire extinguishing compositions are not adapted to changes in the degree of fire hazard of the protected area, the intensity and scale of the fire. These systems extinguish equally regardless of the options for the occurrence of fires and fire development schemes [14] – [16].

Contemporary investigations are focused now on detailed study of membrane systems simulating the basic physical and chemical properties of artificial and natural membranes, including their selectivity to various chemicals, in ionic forms predominantly. In present article the theoretical bases for the development of such sensors with chemo-sensitive surfaces were suggested in continuation of our previous publications [10], [11], [14] – [16].

III. Problem Solution

A. Physical models for the elaboration of detectors of chemical substances in gaze and water phases of artificial or natural origin.

The analyzing detectors with artificial membrane elements have been already developed by the authors [10], [11], [14] – [16]. The scientific basis for such devices with sensor elements could be the set of works on the selective artificial surfaces of various types of glass, sensitive for different chemicals in ionic form. Different versions of such detectors have specific sensitivity for various chemicals, either by own surface or as bed-substrate for covering with the layers of some specific compounds. This physical model of detector can be supported by mathematical model suggested below. They were based on the experiments with the registration of current-voltage characteristics of electrochemical phenomena on the surface of artificial selective membranes as well as selective membranes of living objects. For both types of experiments an adequate physical and mathematical models have to be found. An important preliminary task for mathematical modeling of such phenomena is studying of their physicochemical nature, phenomenon of membranes ionic selectivity both artificial and biological ones. Some types of biosensors as detectors of different biological signals that are transformed further into electrical signals can be constructed in such a way too [10], [11], [13].

B. Modeling of physicochemical phenomena at detector surface.

As theoretical basis we had chosen phenomena of physicochemical interaction of different ions in solutions with glass surfaces. Extremely high specificity of membranes made of glasses of a certain composition with respect to H^+ ions is known from previous publications [14], [15], [19], [20]. Changes in glasses' composition leaded to significant changes in the ion selectivity of membrane glass electrodes, determined under the stationary conditions, as well as changes in the kinetic parameters of such selective membranes [14], [19], [20].

When describing the difference of electric potentials that appear on thin glass membranes (glass electrode) in cases where the latter separate media with different ionic composition, the concepts of ion-exchange equilibrium established at the glass-solution interfaces are most often used. According to the ion-exchange theory of the glass electrode, developed by B. P. Nikol'sky [20], there were supposed the existence of ion-exchange sites and ion exchange processes in the glass material

$$i + \bar{j} \rightleftarrows \bar{i} + j,$$

where i and j are cations in the solution contacting with the glass, $\bar{j}$ and $\bar{i}$ are the same cations bound by fixed negative charges of the glass matrix.

Difference in potentials in this case can be represented by the Nikol'sky equation [20]:

$$\varphi = \frac{RT}{F} In \frac{x_i' + \sum^n k_{ij} x_j'}{x + \sum^n k_{ij} x_j''}, \quad (1)$$

where k is the ion exchange constant. There were

done the assumptions that the ion exchange sites in the glass material are available for any of the exchanging cations, the cation activities in glass are proportional to their molar fractions, and the transmembrane potential difference is determined entirely by the sum of two boundary potential jumps, i.e. the contribution of the diffusion potential can be neglected. The Nikol'sky equation predicts a strictly defined form of transition from one cationic function of membranes to another when the cation composition of one of the media separated by a membrane changes. The experimentally obtained dependence for the region of the transition from one cationic function to another often differs significantly from that predicted by simple ion-exchange theory [20]. To explain this kind of anomaly by Eisenman and co-workers an empirical equation was suggested [20]:

$$\varphi = \varphi^0 + \frac{RT}{F} In\left[x_i^{1/n} + \sum^n \left(K_{ij} x_j \right)^{1/n} \right]^n, \qquad (2)$$

where the value of n is a parameter that determines the degree of non-ideality of the ion-exchange properties of glass.

Unlike the empirical Eisenmann equation, this equation can be successfully used to describe the electrode behavior of glasses in solutions containing three types of cations in cases where a slow transition from one electrode function to another is detected. The latter was registered experimentally during the study of the concentration dependences of the potentials of glass electrodes prepared from sodium aluminum silicate glass (NAS 27.5-4.5) and potassium-gallium glass (KGaS 22-0.7)

These studies have shown that at constant ionic strength of solutions and variable concentrations of H^+, Na^+ and K^+ ions, the constants K'_{HNa} and K'_{HK} as well as a_{HNa} and a_{HK} can be considered as really constant. However, it should be noted that with relatively small ionic forces (10^{-2} – 10^{-3}), the same constants are no longer more could be the constants.

C. Theoretical base for some chemosensitive detectors functioning: glass surface with various chemical compositions.

Interesting feature of glasses used for electrodes production is the ability to obtain different values of cationic selectivity coefficients by varying their chemical composition. In some cases it was possible to register the changes in the potential of the glass electrode with the changes of ionic composition of the solutions that could be attributed to the variability of the cation specificity constants. Besides of this, the cationic selectivity of glass electrodes, which was determined under the steady-state conditions, depends on what solutions were prepared previously (or stored) examined glass electrodes [14], [15], [20].

The classic in this sphere B. P. Nikol'sky and his collaborators obtained theoretically based equations that satisfactorily describe the complex forms of transitions from one cationic function of glasses to another [20]. In particular, the extended transition is well described by the equation

$$\varphi = \varphi^0 + \frac{RT}{2F} In\left(x_i + K'_{ij} x_j \right) + \frac{RT}{2F} In\left(x_i + x_{ij} K'_{ij} x_j \right). \qquad (3)$$

This equation corresponds to the conditions of low dissociation of ionogenic glass groups in their *i*th and *j*th forms.

The constant in this case differs from the constant of Nikol'sky in the equation (1), but it is linked with the latter one by the relation:

$$K_{ij} = K_{ij} x_{ij}^{-1/2},$$

where $x_{ij} = k_i / k_j$ is additional coefficient characterizing the difference in bond strengths of ionogenic groups of the glass with ions *i* and *j*.

Equation (3) can also be extended to the case when three types of cations are present in the solutions [20]:

$$\varphi = \varphi^0 + \frac{RT}{2F} In\left(x_i + K'_{ij} x_j + K'_{ik} x_k \right) + \frac{RT}{2F} In\left(x_i + x_{ij} K'_{ij} x_j + x_{ik} K'_{ik} x_k \right). \qquad (4)$$

Although the question of the cation selectivity dependence of glass electrodes on the concentration of salts in solutions or their ionic strength cannot yet be considered sufficiently investigated, it seems that the specificity decreases significantly with the decreasing of ionic strength to 10^{-3}.

One of the most interesting features of electrode glasses is the ability to obtain different values of cationic selectivity coefficients by varying of their composition [15], [20]. The systems of aluminosilicate glasses (Na_2O (or K_2O) – $A1_2O_3$ – SiO_2) and alumino-borosilicate (Na_2O (or K_2O) – $A1_2O_3$ – B_2O_3 – SiO_2) glasses have been studied in this regard the most comprehensively [20]. The isotherms were found for the first system; they characterized the dependence of K_{ij} constants for

alkali metal cations on the fraction of oxides in the glass.

Systematic studies of such systems and a number of other electrode glass systems, carried out by Eisenman [6] demonstrated that K_{Ki} values and the sequence of alkali metal cations were possible to arrange in the sequences according to the increase of studied coefficients. And these coefficients were linked, consequently, with the function of glass composition. Concerning the latter, from the total 120 possible rearrangements, only 11 different sequences were experimentally detected [20].

During the study of membranes of electrode glasses of various compositions, it was found that the values of their specificity for alkali metal cations can be unambiguously predicted if the value of one of constants of cation specificity, in particular K_{KNa}, is known. Also there were found the dependences of the changes in Gibbs free energy (ΔF_{ij}) for the ion exchange reaction for all alkali metal cations and H^+ ions on the magnitude of the change in free energy of the K^+ and Na^+ ion exchange reaction (ΔF_{KNa}). The equilibrium constant of ion exchange reactions were assumed to be equal to the constants of cation specificity, established by potentiometric determinations, for example, when measuring the values of bi-ionic potentials [20].

$$\Delta F_{ij} = F\varphi_{ij} = -RT \ln K_{ij}. \qquad (5)$$

Eisenman [20] created general theory of ion specificity, applicable both to explain the specificity of ion-exchange materials such as electrode glasses, and the specificity found in the case of liquid ion-exchange membranes and membranes containing cyclic complexing agents. This theory is based on consideration of atomic models of places that hold cations in the membrane or as a result of Coulomb attraction (in the presence of negative charge), or due to ion-dipole interactions (in the case of a neutral group with the dipole moment).

Changes in the free energy during the full exchange reaction between the glass material and the solution (ΔF_{ij}) can be determined if the differences in the internal hydration energies of the ions participating in the exchange process $(E_i - E_j)$, and the differences in internal ion energies in the membrane $(\overline{E}_i - \overline{E}_j)$ are [20]:

$$\Delta F_{ij} = -RT \ln \overline{K}_{ij} (E_i - E_j) - (\overline{E}_i - \overline{E}_j). \qquad (6)$$

The first of the internal energy differences in control [20] can be found on the basis of the tabular data. The difference between the internal energies of cations in an ion-exchange material, such as glass, can be approximated if there is a certain conditional value r, in addition to the crystal radius of the cation, 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 quantity, which characterizes the strength of the anionic field of ion-exchange sites, according to the considered theory determines the ionic selectivity of the membrane.

In the case when the strength of the anionic field of the site that binds the cation in the membrane is small (i.e., the r value is high), of the two cations participating in the exchange process, one that has a greater crystalline radius; because in this case, the difference is less in comparison with the difference, and the latter will determine the preference of the ion transition into the membrane matrix. In this case, the sequence of alkali metal cations arranged in decreasing order of membrane specificity will correspond to the sequence of decreasing crystalline radii [20]:

$$Cs^+ > Rb^+ > K^+ > Na^+ > Li^+ > H^+.$$

At sufficiently small values of r, i.e. a large force of the anion field, of the two above-mentioned differences of the values of internal energies determining the transition of ions into the matrix of the membrane will be the difference of the internal energies of cations in the membrane. In this case, the preference is given to the ions with smaller crystalline radii, which leads to the distortion of the cation sequence just given. There were obtained the isotherms characterizing the specificity of ion exchange with a change in the value of r, and zones corresponding to the already mentioned 11 sequences of alkali metal cations, which are predicted by theory, are indicated [20]. Note that with a gradual increase in the value of r, i.e., with a gradual decrease in the strength of the anion field, the first violation of the sequence is determined by the rearrangement of ions Li^+ and Na^+, which leads to the series $Na^+ >> Li^+ > K^+ > Rb^+ > Cs^+$ (series X). The following rearrangement with a further decrease in the strength of the anion field leads to the fact that the Li^+ ions are already in third place: $Na^+ > K^+ > Li^+ > Rb^+ > Cs^+$ (series IX) [20].

With the opposite direction of changes in the strength of the anion field from its smallest values, i.e. with a gradual decrease in the value of r, the first rearrangement is linked with Cs^+ and Rb^+, concerns the Cs^+ and Rb^+ ions, which gives the $Rb^+ > Cs^+ > K^+ > Na^+ > Li^+$ series (series II). The second rearrangement moves the Cs^+ ions to third place: $Rb^+ > K^+ > Cs^+ > Na^+ > Li^+$ (series III) [20]. It should be noted that the change of series II, III and IV

occurs in a very narrow range of changes in the value of r^- that is, the characteristic "biological" series of permeability of alkali metal cations $K^+ > Rb^+ > Cs^+ > Na^+ > Li^+$ (series IV) with a very small decrease in the field strength is replaced by serie III, in which the first place are the Rb^+ ions [20].

The strength of the anionic field of ion exchange sites in glass is determined by the chemical structure of ion exchange sites and even more – by the state of oxygen atoms. It was demonstrated in numerical publications of Nikol'sky et. al., Eisenman, Belyustin and Schultz, Nikol'sky and Schultz, Schulz et al. [20]. If into the crystal lattice of the main glass former (in particular, SiO_2) the elements that violate this lattice are introduced; and they prevent the polymerization (for example, Na^+, Li^+, etc.), this leads to the appearance of SiO^- groups with high anionic strength and detecting a greater affinity to cations with small crystalline radius. These glasses include the usual H^+-specific samples used to prepare hydrogen glass electrodes. Anionic sites with high ionic strength as a result of hydrolysis can appear on the surface of pure quartz according to Eisenman [20].

When oxides of the type B_2O_3, Al_2O_3 or Ga_2O_3 are inserted into the glass, strong acid groups are formed in these glasses. The binding strength of H^+ ions decreases in this case, the hydrogen electrode function decreases accordingly, and metallic electrode functions are registered. Eisenman, who investigated in detail, as already mentioned, the system of sodium-aluminosilicate glasses, considers that the introduction of Al_2O_3 into the glass composition leads to the appearance of places like $(AlOSi)^-$ – and characterized by relatively low anionic strength. For glasses of the ternary system (for example, sodium-aluminosilicate), an increase in the proportion of oxide Al_2O_3 should lead not only to the appearance of a pronounced metallic function, but also to a gradual transition from lithium-sodium specificity to preferred potassium-cesium specificity. It was registered that the ratio of Na_2O/Al_2O_3 mole fractions started to determine the cation specificity of the glasses.

If we assume that anions F^-, Cl^-, Br^- and I^-, differing in the values of crystalline radii, can to some extent simulate anionic sites in the glass matrix, then it is possible to compare the values at the points corresponding to the crystalline radii of these anions on the isotherms obtained according to Eisenman's theory, with tabular data on the heats and magnitudes of free energies, the formation of halides of various alkali metals in their diatomic gaseous state. Such comparisons, which showed an extremely good agreement between the experimental and calculated values of the energy differences (according to Eisenman), is a strong argument in favor of this theory [20].

On Figure 1 the abscissa axis shows the pH of external solution into which the glass electrode is immersed. On the ordinate axis is the potential difference in the glass electrode circuit, inside of which there was 0.1 M HCl solution. The transitions from the hydrogen to the metal (sodium) electrode function for curve 2 was described by the equation of ion-exchange theory by Nikol'sky. More extended transition from hydrogen to metal (potassium) function, represented by curve 1, can be described by equations (2) or (3).

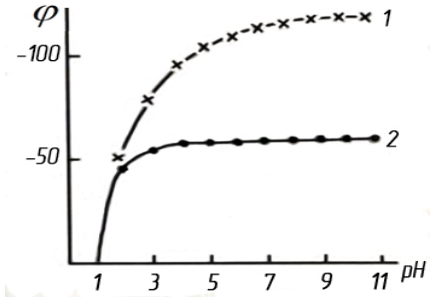

Fig. 1. The dependence of the difference of potential on the membrane for electrode glass NAS 17.5-10 in KCl solutions with pH 0.1 M (curve 1) and NaCl solutions (curve 2) [16], [20] (explanations see in text)

Equation (3) can be successfully used for the description of electrode behavior of glasses in solutions containing three types of cations in cases when the slow transition from one electrode function to another was detected. The latter one was registered experimentally during the study of concentration dependences for the potentials of glass electrodes prepared from sodium aluminum silicate glass (NAS 27.5–4.5) and potassium-gallium glass (KGaS 22–0.7).

These studies have demonstrated that at constant ionic strength of solutions and variable concentrations of H^+, Na^+ and K^+ ions, the constants K'_{HNa} and K'_{HK} as well as a_{HNa} and a_{HK} could be considered as really constant. However, it should be noted that with relatively small ionic forces (10^{-2} – 10^{-3}), the same constants are no longer more could be the constants [20].

IV. CONCLUSIONS

Brief review with the description of information systems (ISs) for the nature protection use was given in present article. Input data for such ISs were input from the detectors incorporated into IS; they were sensitive to harmful chemical molecules in environment. Two main groups of detectors can be

used for such purposes. The first one group included detectors with "biosensor-like" functions, which were sensitive to chemicals like biological objects (cells, their membranes, etc.) [10], [11], [19]. The authors have already developed some versions of ISs with such "biosensor-like" detectors [8] – [11].

Other, the second group of detectors included detectors with surfaces, covered with thin layer, film or membrane with ion-selective properties. They were done in artificial manner, like ion-selective glasses of electrodes [14], [15], [20]. Investigations of the last phenomena were important for understanding of the physico-chemical nature of ion selectivity as well as specificity and selectivity in the broad sense of these terms, since the approximation of such non-isomorphic systems is important in the development of sensory groups for detecting of harmful chemicals in the environment.

The article provides theoretical basis for the development of such sensors with chemo-sensitive surface. Their physical model was suggested as well as mathematical model of phenomena of electrical charges (ions) behavior in membrane vicinity [14] – [16], [20]. The series with different ionic selectivity were proposed on the base of glass surfaces studies. Creation of theoretical bases for the development of device models were directed on the detection of chemical pollutants of environment, especially those released during fires, explosions, other emergencies, including war conditions with a lot of combustion products in the environment in particular, near industrial, chemical enterprises, enterprises of oil and gas cycle, and etc. [14] – [16].

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О. М. Ключко, В. М. Шутко, О. О. Колганова, А. Г. Лізунова, Д. А. Навроцький. Інформаційні технології: фізичні та математичні моделі детекторів для систем моніторингу довкілля

Моніторинг екологічного стану є реальною необхідністю у сучасному світі з його наростаючою тенденцією до антропогенного забруднення навколишнього середовища. Серед таких забруднювачів є хімічні речовини, що виділяються при пожежах, вибухах та інших надзвичайних ситуаціях, при руйнуванні хімічних підприємств, підприємств нафтогазового циклу тощо. Деякі інформаційні системи для відповідного моніторингу коротко описані у цій статті разом із вбудованою гібридною системою електронних детекторів хімічного забруднення навколишнього середовища, які можуть вводити інформацію до таких систем. У попередніх роботах авторів обґрунтовано необхідність розробки двох типів таких детекторів із вказаними властивостями: біосенсорів та детекторів із елементами – штучно створеними селективними мембранами. У даній статті описано саме другий тип детекторів. Запропоновані детектори здатні реєструвати шкідливі хімічні речовини в навколишньому середовищі у повітряній та водній фазах; у основу розробки таких пристроїв покладено теорію мембранних систем. Детектори містили сенсорні елементи, вкриті хемочутливими специфічними покриттями - шарами речовин: мембранами, плівками, тощо. Перебуваючи у контакті з певними хімічними речовинами, ці детектори демонструють властивості хемочутливості та первинної ідентифікації таких сполук. Наведені дослідження були спрямовані на розробку детекторів різних забруднювачів довкілля на основі теорії, яка може бути покладена у основу виявлення таких речовин. Роботи базувалися на глибокому вивченні мембранних систем з подальшою розробкою фізичних та математичних моделей виявлення деяких речовин з урахуванням основних хімічних і фізичних властивостей штучних і природних мембран, а також їх іонної селективності. У статті описано деякі результати математичного моделювання таких детекторів зі штучними мембранами – хемочутливими поверхнями. Підсумовуючи попередній досвід, зроблено короткий огляд публікацій авторів з цих тематик, а також робіт деяких інших авторів. Метою роботи було на основі глибокого вивчення систем штучних мембран запропонувати їх як фізичну модель та узагальнити досвід розробки їх математичних моделей.

Ключові слова: інформаційна система; фізична модель; математична модель; детектор; сенсорний пристрій; пожежі; хімічні речовини; хімічне забруднення навколишнього середовища.

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Е. М. Ключко, В. Н. Шутко, Е. О. Колганова, А. Г. Лизунова, Д. А. Навроцкий. Информационные технологии: физические и математические модели детекторов для систем мониторинга окружающей среды

Мониторинг экологического состояния является реальной необходимостью в современном мире с его нарастающей тенденцией к антропогенному загрязнению окружающей среды. Среди таких загрязнителей есть химические вещества, выделяющиеся при пожарах, взрывах и других чрезвычайных ситуациях, при разрушении химических предприятий, предприятий нефтегазового цикла и т.д. Некоторые информационные системы для соответствующего мониторинга кратко описаны в этой статье вместе со встроенной гибридной системой электронных детекторов химического загрязнения окружающей среды, которые могут вводить информацию в такие системы. В предыдущих работах авторов обоснована необходимость разработки двух типов детекторов с указанными свойствами: биосенсоров и детекторов с элементами – искусственно созданными селективными мембранами. В данной статье описан именно второй тип детекторов. Предлагаемые детекторы способны регистрировать вредные химические вещества в окружающей среде в воздушной и водной фазах; в основу разработки таких устройств положена теория мембранных систем. Детекторы содержали сенсорные элементы, покрытые хемочувствительными специфическими покрытиями – слоями веществ: мембранами, пленками и т.д. При контакте с определенными химическими веществами, эти детекторы демонстрировали свойства хемочувствительности и первичной идентификации таких соединений. Приведенные исследования были направлены на разработку детекторов различных загрязнителей окружающей среды на основе теории, которая может быть положена в основу обнаружения таких веществ. Работы основывались на глубоком изучении мембранных систем с дальнейшей разработкой физических и математических моделей обнаружения некоторых веществ с учетом основных химических и физических свойств искусственных и природных мембран, а также их ионной селективности. В статье описаны некоторые результаты математического моделирования таких детекторов с искусственными мембранами – хемочувствительными поверхностями. Обобщая предыдущий опыт, был сделан краткий обзор публикаций авторов по этим тематикам, а также работ некоторых других авторов. Цель работы заключалась в том, чтобы на основе глубокого изучения искусственных мембранных систем предложить их как физическую модель и обобщить опыт разработки их математических моделей.
Ключевые слова: информационная система; физическая модель; математическая модель; детектор; сенсорное устройство; пожары; химические вещества; химическое загрязнение окружающей среды.

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