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IONOMETRIC METHOD FOR DETERMINATION OF CONCENTRATIONS OF MICROELEMENTS IN RESEARCH OF DIGITAL MEDICINE

Introduction. *The use of ionometric methods of chemical analysis allows to quickly determine the safety of drinking water and the concentration of electrolytes of body fluids in research in digital medicine.*

The purpose of the paper is to develop an algorithm for processing data measuring alkali and alkaline earth metal concentrations by a new electrochemical method of chronoionometry, based on the use of the principles of direct potentiometry and ion-selective electrodes on the inversion chronopotentiometry device.

Methods. *According to the algorithm, the potentials are read in time at a speed of 4 KHz, a constant potential value is determined and a chronopotentiogram is plotted to control stability. According to the linear dependence of the potential difference on the logarithm of the mass of the additives, the mass of the element is found in the sample solution and the values of the element concentrations are determined by the electrode characteristic.*

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Results. The method of chronoionometry was developed and testing was performed on the device of stripping chronopotentiometry "Analyzer SCP" for determining the concentrations of potassium, sodium and calcium in model aqueous solutions. Analytical system "Analyzer SCP" includes five electrochemical research methods: the method of stripping chronopotentiometry (SCP); pulse method SCP (PSCP); differential pulse method SCP (DPSCP); oxidative pulse method SCP (OPSCP); chronoionometric method (CHI). The algorithm for processing concentration measurement data by chronoionometry makes it possible to select specific potential measurements and not take into account unstable values. Measurements are performed by the method of multiple standard additives to ensure controllability of the analysis results.

Conclusions. The proposed method of chronoionometry improves the clarity and control of the stability of potential measurements, allows to choose specific values of additives when calculating concentrations, which increase the reliability and accuracy of measuring concentrations of chemical elements, expands the functionality of the device for stripping chronopotentiometry and makes it more versatile.

Keywords: ionometry method, concentration, ion-selective electrodes, stripping chronopotentiometry, drinking water quality, digital medicine.

INTRODUCTION

One of the priorities of the development and implementation of intelligent information technologies in digital medicine is to improve methods for determining the quality of the human environment for the prevention of the most common diseases.

Most common human diseases are caused by the consumption of poor-quality drinking water and food, as well as the unsatisfactory state of the environment, which necessitates periodic monitoring of these biogeochemical facilities. Of particular importance for the prevention of human diseases is the determination of drinking water quality by measuring low and trace amounts of toxic and man-made chemical elements to establish compliance with physico-chemical and sanitary-toxicological indicators of drinking water safety. Methods of diagnosis include determination of electrolyte concentrations of body fluids, which can be performed by ionometric methods of chemical analysis using ion-selective electrodes.

To perform quality control of the ecological state of the environment, for example, water supply sources [1–3], the International Research and Training Center for Information Technologies and Systems of NAS of Ukraine and MES of Ukraine developed a highly sensitive analytical system "Analyzer SCP" [4], which is based on electrochemical methods of stripping chronopotentiometry SCP. The analytical system allows to determine the trace concentrations of 14 toxic elements in drinking water and in various environmental objects [5–8].

The physical component of SCP chemical methods is the measurement in time of the values of the potential of the indicator and auxiliary electrode in the sample solution, which is a necessary condition for the use of direct potentiometry (ionometry) to determine the concentrations of trace elements. To expand the functionality of the analytical system "Analyzer SCP" added chronoionometric method (CHI) for measuring the concentrations of ions of chemical elements and compounds using ion-selective electrodes (ISE).

PROBLEM STATEMENT

The choice of chemical elements for practical implementation by chronoionometry was determined by the importance of determining the ion concentrations of the element for patient diagnosis by electrolyte analysis, as well as the need to control it in determining the quality of drinking water in accordance with sanitary and toxicological standards.

Based on this, the functions performed in the human body are analyzed, the following common chemical elements: **sodium, potassium, calcium**.

Potassium is the main cation of intracellular fluid, which performs the functions of regulation of neuromuscular excitability, regulation of heart rate, regulation of intracellular and extracellular volume and acid-base status.

The reference range of the concentration of potassium ions (K^+) in serum and blood plasma is (3–12 mmol/dm³). Maintenance of K^+ levels in the human body depends on the normal functioning of the kidneys, gastrointestinal tract, aldosterone excretion in the adrenal glands, the normal acid-base state and the activity of Na^+ / K^+ ions [9].

Violation of any of these mechanisms can alter K^+ levels, so a decrease in blood concentration less than 3.5 mmol/dm³ causes hypokalemia (peripheral paralysis, respiratory failure, cardiac arrhythmia or cardiac arrest) and an increase above 5.0 mmol/dm³ causes hyperkalemia (renal dysfunction, renal failure) [10].

Sodium is the main cation, which makes a significant contribution to the osmolarity of extracellular fluid, and its main function is to regulate water balance and maintain blood pressure [11]. In addition, Na^+ ions play an important role in conducting nerve impulses and activating muscle contraction.

The reference range of concentration of potassium ions (Na^+) is (116–166 mmol/dm³). About a third of Na^+ is in the human body in the form of complexes in the bones; almost all other sodium is dissolved in the extracellular fluid. As a major component of extracellular fluid, Na^+ plays a significant role in maintaining blood volume and blood pressure. If the concentration of sodium in the extracellular fluid is too low and is less than 135 mmol/dm³, then hyponatremia occurs when water moves into the cells, causing them to swell. This is especially dangerous for brain cells, as their expansion increases intracranial pressure, causing brain edema. Causes of hyponatremia can be heart and kidney failure, cirrhosis, Addison's disease, and causes of hypernatremia (sodium concentration greater than 150 mmol/dm³) — chronic renal failure, Conn's syndrome, Cushing's disease, diabetes mellitus. Measurement of Na^+ concentration is especially important for the calculation of the anionic gap, the most important diagnostic parameter in acid-base disorders. Disorders of sodium and water metabolism — dysnatremia is observed in a number of acute and chronic diseases, such as cystic fibrosis, which causes inflammation in the bronchi and leads to hypoxia and pulmonary heart disease [12].

Calcium is one of the most common cations in the body, which plays a key role in bone mineralization and many cellular processes, such as heart and skeletal muscle contraction, neuromuscular transmission, hormone secretion, enzymatic processes such as blood clotting.

The reference range of calcium ion concentrations (Ca^{2+}) is (1.15–1.33 mmol/dm³). Almost all (99%) of the approximately 1 kg of calcium in the human body is contained in bones and teeth, the other calcium is distributed between the intracellular fluid of all cells and the extracellular fluid.

Maintaining Ca^{2+} concentrations in the normal range is important not only for the structural integrity of bones, but also for a number of other physiological functions, including: hemostasis (calcium is a major factor in blood clotting), heart and skeletal muscle contraction, neuromuscular transmission, calcium signaling hormones.

Both increase and decrease in the level of Ca^{2+} are manifested clinically and in severe cases can be fatal. Even a mild disorder, if not detected and corrected, negatively affects the long-term prognosis of the human condition [13].

Ion-selective electrodes for measuring potassium, sodium and calcium.

A large number of different types of ISE have been developed for the determination of potassium, sodium, and calcium ions in biological body fluids, ecological objects of the environment and technological production processes. When using ISE, the main directions of research are aimed at increasing the selectivity of individual ions [14, 15], the use of polymer composites [16, 17], carbon nanotubes and nanomaterials [18, 19], nanowire transistor sensors [20], flexible ion sensors based on polyelectrolyte layers assembled on carbon adhesive tape [21], highly stretchable potentiometric ion sensor based on surface strain redistributed fiber for sweat monitoring [22], wearable potentiometric sensors based on commercial carbon fibres [23]. ISE determination of concentrations for each specific ion has specific features caused by the subject: the use of nanostructured TCNQ for ion-selective K^+ and Na^+ electrodes [24], the use of flash chronopotentiometry at polymer membrane ion-selective electrodes to measure total calcium [25], introduction of new linkers for sodium selective potentiometric sensors [26].

For researching an ecological condition of objects of environment use ISE measuring, which are serially issued, for example, "ELIS-121K", "ELIS-112Na", "ELIS-121Ca", and comparative silver chloride electrodes standard or with a double electrochemical key, for example, electrode "Esr-10101".

Ion-selective automated systems measurement of potassium, sodium and calcium. To determine the concentrations of K^+ , Na^+ and Ca^{2+} ions in the electrolytes of body fluids, bioanalyzers and spectrometers of various designs are mainly used, for example, Agilent 2100 bioanalyzer and Agilent 7500 ICP-MS spectrometer (Hewlett-Packard), bioanalyzers DS-261, DS-401, BS3000M (Dialab, Austria) and others. Specialized systems for measuring potassium using an array of ion-selective electrodes controlled by a microcomputer [27], sodium in a wireless ion-selective electrode system [28, 29], total sodium and potassium in surface and groundwater using a flame photometer [30], for real-time ion monitoring [31] and many others.

To ensure control of the concentrations of these chemical elements in the investigated solutions, it is necessary to increase the reliability and accuracy of determining their concentrations. Since the performance of electrochemical studies and determination of concentrations of chemical elements: sodium, potassium, calcium, is the most relevant for the tasks of determining the quality of drinking water, the task was to develop methods and algorithms for determining these elements in drinking water.

The purpose of the paper is to develop a method and algorithm for processing data measuring alkali and alkaline earth metal concentrations for a new electrochemical method of analysis — chronoionometry, the principle of which is based on the application of direct potentiometry on the device for inversion chronopotentiometry.

FUNDAMENTALS OF THE CHRONIONOMETRIC METHOD OF DETERMINATION OF CONCENTRATION

The method of ionometry is based on the principle of potentiometric analysis, according to which the measurement of the potential difference (electromotive force — EMF) between the electrodes is carried out. The essence of the method is to determine the activity (concentration) of ions in the mode of direct potentiometry using measuring ISE and comparative silver chloride electrodes. During operation, ISE selectively responds to a certain type of ions, and there is a linear dependence of the EMF of the electrode system on the concentration of ions, according to the Nernst equation [14].

Determination of the concentrations of the elements in the solution is carried out by the method of calibration graph or additives of a standard solution of ions of the element. The main disadvantage of the calibration graph method is the significant complication of the process of reproducibility of the analysis results, which requires constant conditions for calibration, validation and measurement of the ionic strength of the solution.

The method of additives is more reliable and accurate. Depending on the type of processing of the results of ion concentration measurements, the standard additive method or the Gran method are used [32]. The disadvantages of these methods are the use in the formulas for calculating the concentration of the steepness of the electrode function of the calibration graph, which requires its prior careful construction or solution of certain transcendental equations. In practice, the method of multiple additives (SBD) of a standard solution of element ions with the calculation of concentrations by the Gran method using the steepness of the obtained linear electrode function of the calibration graph and the values of the mass of additives.

On the device for measuring the parameters of aqueous solutions [33], implemented on the "Analyzer SCP", the process of determining the potentials by chronoionometric analysis is performed as follows. During the measurement, an electrolyzer with a sample solution is used, which is installed on a magnetic stirrer, with constant slow stirring of the solution. At a speed of 4 KHz read the values of potentials in the measurement cycle lasting one second for a given period of measurement time T . In this case, in the first half of the cycle the signal is stored, and in the second half of the cycle the obtained values are processed and determined by the potential E in the cycle measurement. The obtained values of $E(t)$ in real time in the form of chronopotentiograms are displayed (Fig. 1), which allows to monitor the process of determining the constant potential and allows to increase the reliability of determining the concentrations of element ions in the sample solution.

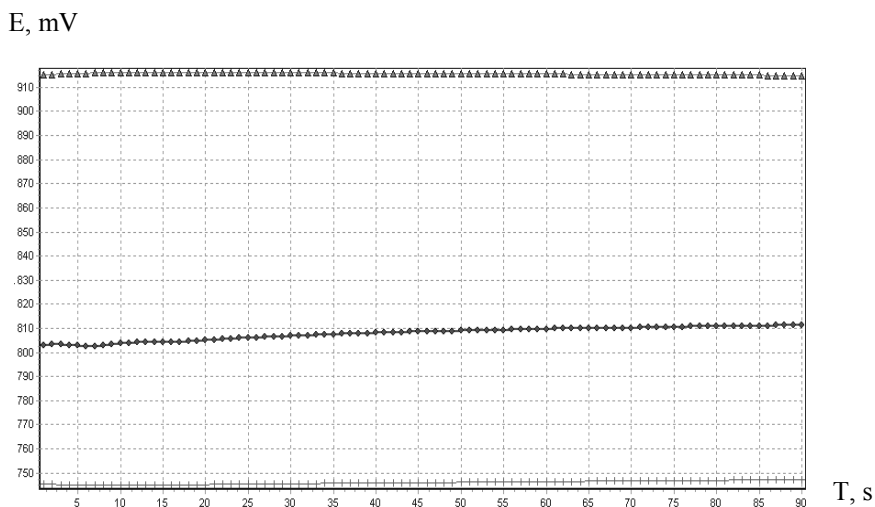


Fig. 1. Chronopotentiogram of potassium ion potential measurement

ALGORITHM OF DATA PROCESSING BY THE METHOD OF CHRONIONOMETRY

The developed algorithm consists of five steps: construction of a linear calibration graph at two points; measuring the potential in the sample solution; determination of the mass of the additive; measuring the potential in the sample solution with the additive and calculating the concentration by the method SBD.

To describe the features of the proposed algorithm, consider measuring the concentration of potassium ions in a model solution of potassium chloride: a standard solution of $C_{KCl} = 1 \cdot 10^{-4}$ M KCl mol /dm³ with a concentration of potassium ions $C_K = 3.91$ mg/dm³.

Step 1. Construction of a linear calibration graph at two points. When determining the concentration by the method of multiple standard additives, the calibration graph is based on two values of the extreme points of the ISE measurement range. Thus, to determine the concentration of potassium ions C_K use calibration solutions of $1 \cdot 10^{-5}$ and $1 \cdot 10^{-2}$ M KCl mol/dm³, measuring ion-selective electrode and silver chloride electrode with a double electrolytic key. During the time $T = 60$ s, the chronopotentiogram $E(t)$ is read and displayed. According to the values of the potentials of the endpoints of the chronopotentiogram, a calibration graph is constructed at two points to determine the concentration of the KCl solution (Fig. 2).

The vertical line shows the maximum permissible value (MPV) of potassium in drinking water ($MPV_K = 20$ mg/dm³, $pK = -\lg C = 3,29$), which allows a qualitative visual assessment of ion concentrations in the sample solution.

According to the calibration graph, the steepness of the electrode function S of the linear dependence $E = E_0 + S \cdot pC$ of the potential change from the ion activity index $pC = -\lg C$ is calculated.

For this example, the equation of the linear electrode characteristic (1) is obtained in the form: $E = 1046.2 - 53.75 \cdot pK$, the inverse linear equation will be: $pK = 19.246 - 0.0186 \cdot E$.

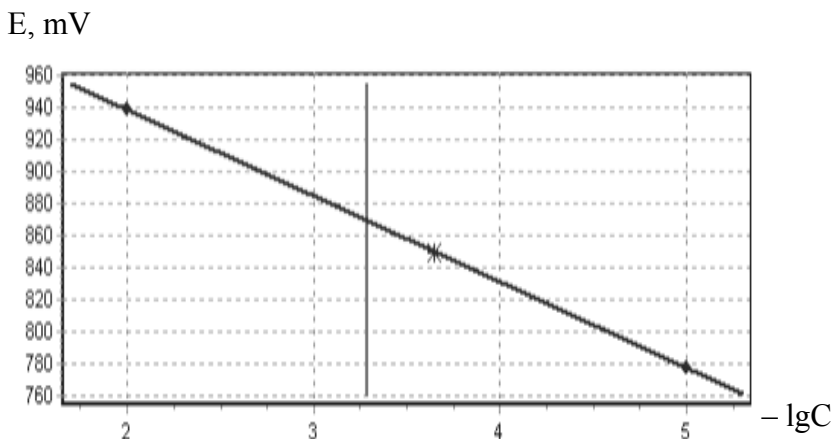


Fig. 2. The calibration curve for the two points

Step 2. Measurement of the potential in the sample solution. Perform measurement of the constant value of the potential of the model solution $C_{\text{KCl}} = 1 \cdot 10^{-4}$ M KCl with constant stirring for a given time of measurement T and calculate the inverse equation of the electrode characteristics of the molar concentration of the solution $C_{\text{KCl}} = 10^{-pK}$ (mol/dm³), mass concentration ion $C_K = M \cdot 10^{-pK}$, where M is the molar mass of the potassium ion (39100 mg/dm³), and reflect the sign "*" in Fig. 2.

For our example we obtain: sample potential $E_S = 850$ mV; $pK = 3.65$, which corresponds to the concentration of potassium ions $C_K = 8.76$ mg/dm³ and the molar concentration of the model solution $C_{\text{KCl}} = 2.24 \cdot 10^{-4}$ M KCl. The result of measuring potassium ions in the model solution according to the calibration graph at two points was obtained with a significant relative error.

Step 3. Determining the weight of the additive. Based on the value of C_{KCl} determine the concentration of the standard solution and the corresponding mass of the addition of ions of the element so that it was half-order or an order of magnitude greater. For a model sample with a volume of 10 cm³ the concentration of the standard solution of the additive will be $C_{\text{KCl}} = 1 \cdot 10^{-2}$ M KCl, which corresponds to the mass of the addition of potassium ions $M_K = 391$ μg.

Step 4. Measurement of the potential in the sample solution with the additive. Add sample M_K standard solution of potassium ions to the solution and determine the constant value of the sample potential with the additive, repeating the measurement process for five additives, without changing the volume and weight of the additive. If the potential values in the sample or the sample with the additive are unstable, the measurement is repeated.

Step 5. Calculation of concentration by the method of multiple additives. According to the measurement results, the values of the potential difference between the potential are formed E_{Addj} of the current additive and the average potential E_S of the sample: $\Delta E_j = E_{\text{Addj}} - E_S$, which correspond to the increasing values of the mass of the ion additive $M_j = M_{j-1} + M_K$ in solution samples with additives. The values of ΔE_j and $(-lgM_j)$ are processed by the method of least squares, the direct and inverse linear dependence of the potential difference on the logarithm of the additive mass is obtained. According to the order of

processing the results of measurements of concentrations by the method of Gran, the obtained linear graph is extrapolated to the intersection with the abscissa and determine the value $(-\lg M_S)$, which corresponds to the initial concentration of ion element M_S in the sample solution without additives. The graph of the linear dependence of the potential difference from the logarithm of the mass for the five additives is shown in Fig. 3.

The values of the additive mass M_i are corrected by increasing them by the value of the ion mass of the element $M_j = M_j + M_S$, to obtain the actual ion mass when measuring the sample with the additive.

Calculate the concentration of ions of the element $C_j = M_j / V$ according to the values of the mass M_j and the volume of the solution of the sample V (for example, 0.01 dm^3) for the sample C_S and the sample with the addition of C_{Adj} .

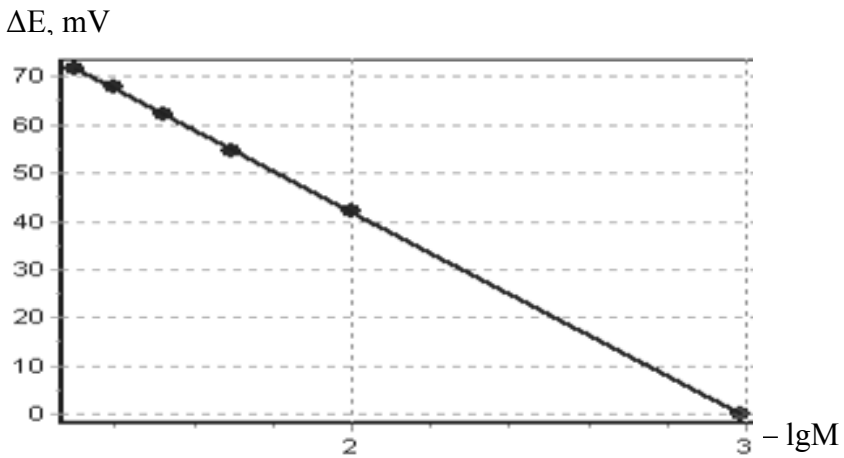


Fig. 3. Dependence of the potential difference on the logarithm of the mass for five additives

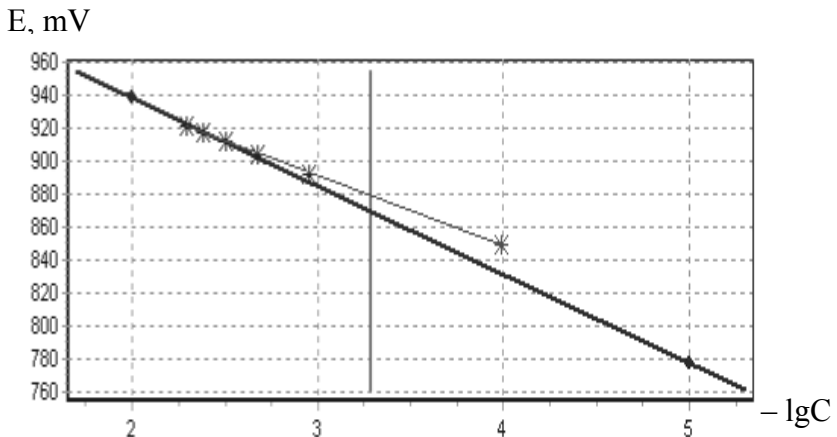


Fig. 4. Electrode characteristic of potassium concentration measurement for five additives

Using the measurement potentials E_S , E_{Adj} and the values of C_S , C_{Adj} are calculated by the method SBD, the coefficients of the forward and inverse linear electrode characteristics of the measurement of element ions by the method of multiple standard additives. The graph of the electrode characteristics for the five additives is shown in Fig. 4.

For our example of measuring potassium ions with five additives, the electrode characteristic will be written as: $E = 1018.3 - 42.30 \cdot pK$, and the inverse relationship will be: $pK = 24.071 - 0.0236 \cdot E$. The inverse relationship for sample potential $E_S = 850$ mV the concentration of potassium ions will be $C_K = 4.01$ mg/dm³, the molar concentration of the solution $C_{KCl} = 1,027 \cdot 10^{-4}$ M KCl. Thus, the result of measuring the concentration by chronoionometry by the method of multiple standard additives was determined with a relative error of 2.7 %, which is much better than the result obtained by the calibration graph.

The algorithm for processing concentration measurement data by chronoionometry has the ability to select specific potential measurements and not take into account unstable potential values. Choose to calculate the concentration of only the first three additives, then the dependence of the electrode characteristic will be $E = 1015.8 - 41.52 pK$, and the inverse dependence $pK = 24.464 - 0.0241 \cdot E$. The graph of the linear dependence by the Gran method is shown in Fig. 5 and a graph of the electrode characteristics for the three additives is shown in Fig. 6.

For the sample potential $E_S = 850$ mV concentration of potassium ions will be $C_K = 3.91$ mg/dm³ and the molar concentration of $C_{KCl} = 1.001 \cdot 10^{-4}$ M KCl. The result of measuring the concentration by the method of chronoionometry with three additives was determined with a relative error of 0.1%, which is better than the previous results.

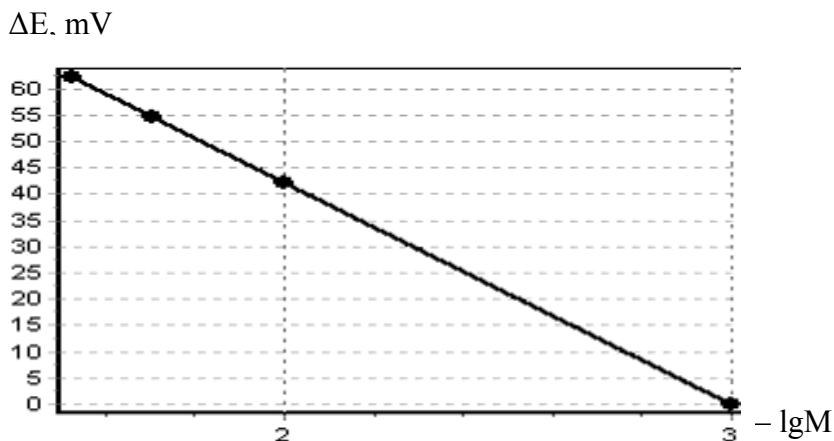


Fig. 5. Dependence of the potential difference on the logarithm of the mass for three additives

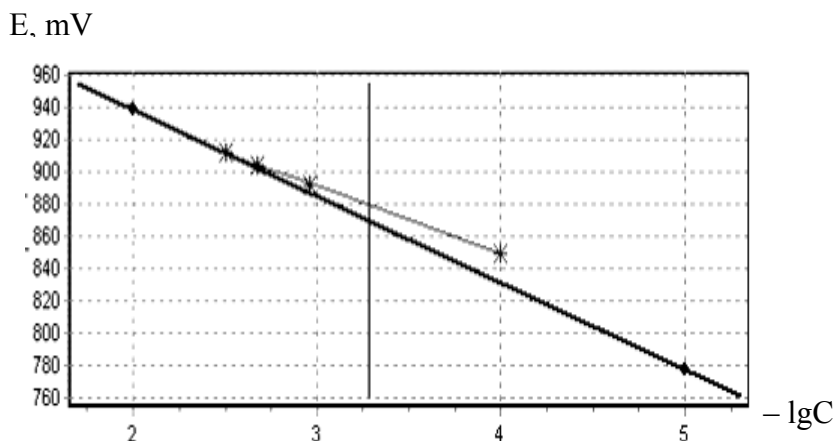


Fig. 6. Electrode characteristic of potassium concentration measurement for three additives

Performing measurements by the method of multiple standard additives improves the controllability of the analysis results, increases the reliability and accuracy of determination of concentrations.

IMPLEMENTATION OF THE ALGORITHM IN INFORMATION TECHNOLOGY AND CONCENTRATION MEASUREMENT DEVICES

To measure the potentials, a high resistance was added to the reading channel and an auxiliary chlorine-silver electrode with a double electrolytic key was developed, which showed better characteristics for the CHI method compared to the electrode "Esr-10101".

The analytical system "Analyzer SCP" includes a total of five electrochemical research methods: the

- stripping chronopotentiometry (SCP),
- pulse stripping chronopotentiometry (PSCP) [4],
- differential pulse stripping chronopotentiometry (DPSCP),
- oxidative pulse stripping chronopotentiometry (OPSCP),
- chronoionometric method (CHI) [33].

The developed data processing algorithm for the new chronoionometric method of analysis is implemented in the form of a subsystem, which has become an integral part of the information technology software of the device "Analyzer SCP".

The results of measuring the concentrations of chemical elements by the method of chronoionometry and auxiliary parameters: the value of ion activity to determine their relationship with the concentration of elements at points in the measurement range and other ISE parameters; coordinates of calibration points of calibration graphs of ISE — all these values are stored in the general database of information technology that considerably accelerates adjustment of the device before the beginning of measurement of concentrations.

The main window of the subsystem for determining concentrations by the method of chronoionometry is given in Fig. 7.

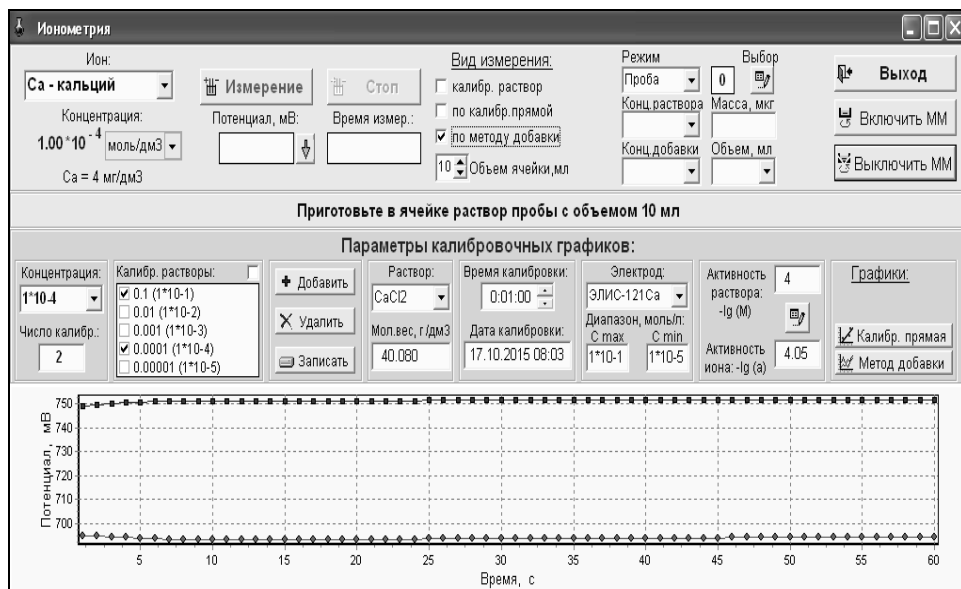


Fig. 7. The main window of the program for determining the concentrations of chemical elements by chronoionometry (Calibration curves for measuring calcium)

The subsystem implements two approaches to determining concentrations by chronoionometry:

1. The method of calibration graph.
2. The method of reusable standard additives.

The use in one device of determining the concentrations of toxic elements by the methods of SCP, PSCP, DPSCP, OPSCP and the new method CHI allows to significantly expand the number of chemical elements analyzed. At the same time, for the method of chronoionometry the clarity of the research is increased, the control of the measurement stability is improved by taking into account the statistically large number of potential values read from the ISE. The calculation of the electrode characteristic by the method of multiple standard additives and its display together with the calibration graph, as well as the ability to select the required potentials of the additive to calculate concentrations, all significantly improves the process of measuring concentrations compared to existing technologies in ionometry.

The use of these methods allows the "Analyzer SCP" to measure the concentration of 17 chemical elements (Hg, As, Pb, Cd, Cu, Zn, Sn, Ni, Co, Se, Mn, I, Cr, Fe, K, Na, Ca) in the environment and in drinking water. The use of the CHI method allows to determine the content of K, Na and Ca without sample preparation, which significantly increases the expressiveness and ease of analysis of these elements.

The results of measuring the concentrations of chemical elements and auxiliary parameters of the CHI method: the value of ion activity to determine their relationship with the concentration of elements and other parameters of ISE; the coordinates of the calibration points of the calibration graphs of the electrodes are stored in the general database of the device, which significantly speeds up its adjustment before the measurement of concentrations. At the same time, the visibility increases and the control of measurement stability is improved by taking into account a statistically large number of potential values read from the electrodes.

The calculation of the electrode characteristic by the method of multiple standard additives and its display together with the calibration graph, as well as the ability to select the required additive potentials for calculating concentrations, all significantly improves the measurement process compared to existing technologies in ionometry.

To determine the concentrations of K^+ , Na^+ , Ca^{2+} ions in water, methods for measuring chemical elements have been developed, confirmed by patents: a device for determining the concentration by CHI [33], a method for determining calcium in aqueous solutions [34], sodium [35] and potassium [36]. These methods have significant scientific value for the development of electrochemical methods of analysis, and can also be used in chemical technology, biotechnology and environmental analysis.

The effectiveness of the described chronoionometric method for determining the concentrations of trace elements potassium, sodium and calcium in drinking water is proved by comparison with the characteristics of analytical systems developed in other countries.

ANALYSIS ACCURACY ALGORITHM MEASUREMENT OF CONCENTRATIONS CHRONOIONOMETRYCHNYM ANALYSIS METHOD

In accordance with hygienic standards, assessment of safety and quality of drinking water is carried out according to epidemic safety indicators, sanitary-chemical and radiation indicators. The main principle of practical implementation of chronoionometry methods in determining the quality of drinking water is that the measurement should provide a reliable determination of the concentrations of chemical elements below the maximum allowable concentrations of MPV.

Table 1 shows the normative values of the MPV in Ukraine for chemical elements and ranges of measurement of concentrations, according to the methods of measurement in water: 1 — tap; 2 — from wells and catchments of springs; 3 — packed up from filling points, ditches; 4 — water of the central drinking water supply; 5 — water of non-central drinking water supply.

At low levels of physiological value of the mineral composition of drinking water (below the minimum limit of optimal value) packaged drinking water (at bottling points) can be treated, but within the limits specified in Table 1.

In the process of preparation of methods for measuring potassium, sodium and calcium ions in water, a study was conducted and the relative errors of concentration measurements were calculated for the series of additives to model solutions, which indicate the accuracy of concentrations by chronoionometry (Table 2).

According to the above data, the relative measurement error of the concentration of potassium, sodium, calcium ions in water is in the range of values from 2.4 % to 16.4 %, which is less than the normalized relative measurement error of 20 %.

Methodological support for measuring the concentrations of potassium, sodium, calcium ions by chronoionometric method in cooperation with the International Research and Training Center for Information Technologies and Systems of NAS of Ukraine and MES of Ukraine and the National University of Life and Environmental Sciences of Ukraine [37].

Table 1. Sanitary and chemical indicators of safety and quality of drinking water

Element	Maximum concentration limit for drinking water (mg/dm ³), no more than					Optimal value within ³⁾ , mg/dm ³	Measurement ranges "Analyzer SCP" mg/dm ³
	1 ¹⁾	2 ¹⁾	3 ¹⁾	4 ²⁾	5 ²⁾		
Potassium (K)	-	-	-	-	20	2 – 20	0,4 – 3900
Sodium (Na) ⁴⁾	200	-	200	200	200	2 – 20	2,3 – 2300
Calcium (Ca)	-	-	130	-	130	25 – 75	0,4 – 4100

Notes:

¹⁾ DSanPiN 2.2.4-171-10 "Hygienic requirements for drinking water intended for human consumption"

²⁾ DSTU 7525: 2014 Drinking water. Requirements and methods of control (water of centralized and decentralized drinking water supply)

³⁾ Optimal values of indicators of physiological completeness of mineral composition of drinking water

⁴⁾ Substances of the II class of danger (degree of danger to the person of chemical substances polluting water depending on their toxicity, limiting signs of harm and the ability to cause adverse long-term effects)

Table 2. Parameters and errors of measurements of elements in model solutions

№ samples	Set concentration		Results		
			Measured concentration		Relative error
	mol/dm ³	µg/cm ³	mol/cm ³	µg/cm ³	%
1	2	3	4	5	6
Potassium (K)					
	KCl	K ⁺	KCl	K ⁺	2.7
1	0.0001	3.91	0.0001027	4.01	2.7
2	0.001	39.1	0.001052	41.1	5.2
3	0.01	391.0	0.00889	347.6	11.1
Sodium (Na)					
	NaCl	Na ⁺	NaCl	Na ⁺	
1	0.0001	2.3	0.000111	2.55	11.0
2	0.001	23.0	0.001024	23.6	2.4
3	0.01	230.0	0.00836	192.2	16.4
Calcium (Ca)					
	CaCl	Ca ²⁺	CaCl	Ca ²⁺	
1	0.0001	4.008	0.0000962	3.85	3.8
2	0.001	40.08	0.001077	43.2	7.7
3	0.01	400.8	0.00880	352.8	12.0

Potential consumers analytical system "Analyzer SCP" are:

- control and diagnostic laboratories Ministry of Agriculture, Ministry of Health, Ministry of Environment and Natural Resources,
- laboratories of quality and certification of agricultural products,
- control and production laboratories of food industry enterprises,
- centralized water supply laboratories,
- educational and scientific chemical and ecological laboratories of educational institutions,
- laboratories of product quality.

The proposed technology for measuring the concentrations of potassium, sodium and calcium in water can be used to determine the concentrations of electrolytes in the study of body fluids (whole blood, serum, plasma, urine).

CONCLUSIONS

The main principle of practical implementation of chronoionometry methods during toxicological research is reliable measurement of potassium, sodium, calcium ions in determining the safety of drinking water and human quality for the prevention of the most common diseases, the use of biological fluids in digital medicine and study of possibilities of improvement of methods of diagnostics of the person with use of results of the analysis of ions of other toxic chemical elements and connections.

Validation of the methodology and verification of the analytical system "Analyzer SCP" showed that they fully meet the technical and regulatory requirements and are suitable for quantitative determination of the mass concentration of potassium, sodium, calcium ions in drinking water and water of various natural origin.

The developed method of chronoionometric measurement of ions in different media can be extended to other chemical elements: fluorine, chlorine, nitrates, ammonium and other inorganic and organic compounds for which there are ion-selective electrodes.

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ІОНОМЕТРИЧНИЙ МЕТОД ВИЗНАЧЕННЯ КОНЦЕНТРАЦІЙ МІКРОЕЛЕМЕНТІВ У ДОСЛІДЖЕННЯХ ЦИФРОВОЇ МЕДИЦИНИ

Вступ. Використання іонометричних методів хімічного аналізу дає змогу швидко визначити безпечність питної води та концентрації електролітів біологічних рідин організму у дослідженнях цифрової медицини.

Мета статті — розробити алгоритм оброблення даних вимірювання концентрацій лужних та лужноземельних металів новим електрохімічним методом хроноіонометрії, оснований на використанні принципів прямої потенціометрії та іон-селективних електродів на приладі інверсійної хронопотенціометрії.

Методи. Згідно з алгоритмом на приладі зчитують потенціали у часі зі швидкістю 4 КГц, визначають стає значення потенціалу та виводять графік хронопотенціограми для контролю стабільності. За лінійною залежністю різниці потенціалів від логарифма маси добавок знаходять масу елемента у розчині проби та визначають значення концентрації елемента за електродною характеристикою.

Результати. Розроблено метод хроноіонометрії та проведено тестування на приладі інверсійної хронопотенціометрії «Аналізатор ІХП» визначення концентрацій калію, натрію та кальцію в модельних водних розчинах. Аналітична система «Аналізатор ІХП» включає п'ять електрохімічних методів дослідження: метод інверсійної хронопотенціометрії SCP (stripping chronopotentiometry); імпульсний метод PSCP (pulse SCP); диференційний імпульсний метод DPSCP (differential pulse SCP); окислювальний імпульсний метод OPSCP (oxidative pulse SCP); хроноіонометричний метод СНІ (chronopotentiometric method). Алгоритм оброблення даних вимірювання концентрації методом хроноіонометрії надає можливість виконувати вибір конкретних вимірювань потенціалів та не враховувати нестабільні значення. Виконання вимірювань здійснюється шляхом багаторазових стандартних добавок для забезпечення контрольованості результатів аналізу.

Висновки. Запропонований метод хроноіонометрії покращує наочність та контроль стабільності вимірювання потенціалів, дає змогу вибрати конкретні значення добавок для розрахунку концентрацій, що підвищує надійність та точність вимірювання концентрацій хімічних елементів, розширює функціональні можливості приладу для інверсійної хронопотенціометрії та робить його більш універсальним.

Ключові слова: метод іонометрії, концентрація, іон-селективні електроди, інверсійна хронопотенціометрія, якість питної води, цифрова медицина.