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METHOD OF CHRONOIONOMETRIC DETERMINATION OF CONCENTRATIONS OF FLUORINE, NITRATE, AMMONIUM IN DRINKING WATER

Introduction. *Using method of chronoionometry and ion-selective electrodes makes it possible to determine quickly the concentrations of chemical elements, which allows you to assess the quality of drinking water and the ecological condition of the environment.*

The purpose of the paper is to apply the developed method of chronoionometry to measure the concentrations of fluoride, nitrate, ammonium in drinking water and to assess the accuracy of measuring concentrations.

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Methods. Chronoionometric method of chemical analysis uses the principles of direct potentiometry to measure the concentrations of chemical elements.

Results. Methods for detection the concentrations of fluorine, nitrates, ammonium in drinking water were obtained and tests were performed in model aqueous solutions using the device of inversion chronopotentiometry "Analyzer SCP", which testify to the compliance of measurement errors with metrological normative values.

Conclusions. Improved analytical system "Analyzer SCP" to determine the concentration of 20 chemical elements (Hg, As, Pb, Cd, Cu, Zn, Sn, Ni, Co, Se, Mn, I, Cr, Fe, K, Na, Ca, F, NO₃, NH₄) in aqueous solutions by inversion chronopotentiometry and chronoionometry, which is sufficient for ecological assessment of drinking water quality and environmental objects. The use of a new method of chronoionometry significantly expands the functionality of the device of inversion chronopotentiometry, increases the reliability and accuracy of measuring the concentrations of chemical elements.

Keywords: chronoionometry method, concentration, of fluoride, nitrate, ammonium, ion-selective electrode, inversion chronopotentiometry, drinking water.

INTRODUCTION

At the present stage of development of society, one of the central places is occupied by the problems of the ecological state of the environment and its pollution by various toxic chemical elements. Therefore, much attention is paid to the control of quality and safety of drinking water and food with the help of cost-effective and highly accurate means of control. According to the WHO, more than 80 % of human diseases can be caused by drinking contaminated water. It is known that the daily human need for water is 2.5–3.0 liters. Along with drinking water, heavy metals, microelements, as well as many salts and macronutrients, in particular, fluoride compounds, nitrate, and ammonium enter the human body.

Therefore, there is a need to develop intelligent methods and tools for environmental monitoring, the introduction of modern information technology that will provide versatility and expressive measurement of concentrations of chemical elements. Such technologies make it possible to obtain, collect and intelligently analyze the obtained environmental information for decision-making on the prevention of human health disorders and carrying out preventive ecological measures.

Thus, in order to perform quality control and assess the ecological state of the environment, primarily water supply sources [1], the International Research and Training Center for Information Technologies and Systems of NAS of Ukraine and MES of Ukraine has developed a highly sensitive analytical system "Analyzer SCP" on the use of electrochemical methods of inversion chronopotentiometry (SCP) and a new chronoionometric method of analysis (CHI).

The analytical system makes it possible to determine in drinking water and in the environment trace concentrations of 17 chemical elements [2], including such ions as potassium (K⁺), sodium (Na⁺) and calcium (Ca²⁺), measured by chronoionometric by the method using ion-selective electrodes ISE (ion-selective electrodes). The application of the CHI method allowed to increase the accuracy of the ionometric study and to improve the stability of the potential measurement.

According to the current normative document in Ukraine on the quality of drinking water intended for human consumption [1], in addition to determining the content of heavy metals (Hg, As, Pb, Cd, Cu, Zn, Sn, Ni, Co, Mn, Cr, Fe) and elements (Se, I, K, Na, Ca) it is necessary to determine a number of sanitary and toxicological indicators: ammonium NH₄⁺, nitrate NO₃⁻ and fluorides F⁻ (hazard class II). The concentration of these macronutrients in drinking water can also be

measured on the device "Analyzer SCP", using our developed method CHI [2, 3], information technology [4] and the corresponding ISE [5], which will expand the functionality of the device.

PROBLEM STATEMENT

The content of fluorine ions, nitrates and ammonium in water has a significant affected human health, so it is important to control them in accordance with sanitary and toxicological standards with the help of modern analytical instruments, fluoride (HF) by passive diffusion [6].

According to the state standards which include the method of CHI.

Fluoride is one of the most important chemical elements that significantly affects human life in general. The daily intake of fluoride anions with food is on average 2–3 mg 90–97 % of which is absorbed in the gastrointestinal tract and blood, from blood plasma fluoride ions are rapidly distributed in intracellular and extracellular fluids, tissues and organs, they are able to penetrate quickly. through biological membranes in the form of hydrogen, the permissible concentration of fluoride in drinking water is 1.5 mg/dm³ [1]. At concentrations less than 0.7 mg/dm³ there is a deficiency of fluoride, i.e. hypofluorosis. It provokes the development of caries, most children are prone to it. There are also conventional guidelines for the association of hypofluorosis with rickets, impaired immune status and disorders of calcium metabolism [7].

Increasing the concentration of fluoride in drinking water to 2 mg/dm³ causes the spread of fluorosis and increases the severity of its course. If the concentration is higher than acceptable (1.5–2 mg/dm³), then 30–40 % of the population is affected by dental fluorosis, mainly I and II degree. The use of water with such a concentration of fluoride may be temporarily acceptable in terms of local water supply [8, 9]. In the case of centralized water supply, it is necessary to carry out defluoridation or dilution of water. At high concentrations of fluoride in drinking water (2–6 mg/dm³) the incidence of fluorosis is 30–90 %, and 10–50 % of them have fluorosis of III–IV degree [10]. Among children, there are often cases of developmental delay and bone mineralization [11]. In some people who drink water with a fluoride content of 4–6 mg/dm³, there is an increase in bone density and impaired conditioned reflex activity.

At very high concentrations of fluoride in drinking water (6–15 mg/dm³ and more) 90–100 % of the population becomes affected by dental fluorosis with a predominance of severe forms, significantly increased fragility of teeth, mineralization disorders and changes in bones by type of osteosclerosis [12]. There is suppression of thyroid function, changes in the activity of certain enzyme systems of the blood, changes in the myocardium, inhibition of bioelectrical activity of the brain, as well as disorders of other internal organs (e.g. liver), which are detected during functional examination [13].

Fluoride in minimal amounts is necessary for metabolic processes in the body and is the seventh vital trace element after copper, zinc, iron, manganese, iodine and cobalt [14]. Fluoride has a regulatory effect not only on bone cells (osteoblasts and osteoclasts), but also on cells of the endothelium, liver, kidneys, myocardium and nervous system. Excretion of fluoride from the body occurs through the skin, digestive tract and urinary system with an excretion period of 2 to 9 hours. At the cellular level under the action of fluoride in the cells increases the generation of O₂,

H₂O₂, OH⁻ and nitric oxide NO. Fluoride compounds have been shown to be a cytotoxic factor involved in metabolic alteration, modulation of intracellular signaling pathways and activation of programmed cell death. The mechanisms of physiological or toxic effects of fluoride compounds on the body depend on their concentrations and duration of consumption [15].

Nitrate is inorganic anions (NO₃⁻), which are formed due to oxidation of elemental nitrogen. It is an important nutrient for the synthesis of plant proteins, which plays a significant role in the nitrogen cycle of soils and water. Nitrate is formed by natural biological and physical oxidation, they are ubiquitous in the environment [16]. Most nitrate come from inorganic chemicals, especially from fertilizers produced for agriculture. Ammonia from livestock waste can be oxidized to nitrate by soil bacteria under aerobic conditions. It can also be a significant source of nitrate in surface and groundwater, especially near areas where animals are raised [17].

The primary toxic effect of the inorganic nitrate ion (NO₃⁻) is due to its reduction to nitrite (NO₂⁻). Organic nitrate is metabolized in the liver, which leads to an increase in nitrite in the blood. Nitrate and nitrite are excreted mainly in the urine as nitrate. The main toxic effect of inorganic nitrate is the oxidation of iron in hemoglobin due to an excess of nitrites that form methemoglobin. Infants under 6 months of age make up the most sensitive population. Epidemiological studies have shown that infant formula prepared from drinking water with a nitrate nitrogen content of more than 10 mg/dm³ can lead to methemoglobinemia, especially in children under 2 months of age [18]. The results show a correlation between the number of congenital malformations of the central nervous system, musculoskeletal system and infants with the amount of inorganic nitrate in drinking water that was consumed. Elderly people, people with anemia, people with respiratory and cardiovascular diseases are also sensitive to nitrate. There are cases of the disease in older children (after consuming water with a high content of nitrate).

Therefore, it is strictly forbidden to use water from wells and catchments where the nitrate content exceeds the norm. Boiling nitrate-contaminated water does not reduce, but increases its toxicity by 39–86 %. Therefore, it is important to determine the nitrate content in drinking water in a timely manner, using analytical measurement methods [19–22].

Organic nitrate is well known for their vasodilating action and is used to treat angina. The possible carcinogenicity of nitrate depends on the conversion of nitrate to nitrite and the reaction of nitrite with secondary amines, amides and carbamates to form carcinogenic nitro compounds.

Ammonium — a substance that is the initial product of decomposition of organic nitrogenous substances, is readily soluble and is always present in water in small concentrations as a mandatory component. Ammonium appears in water due to the dissolution of ammonia in it [23].

Ammonium is one of the most important cations for monitoring, especially in wastewater areas, as large amounts can be toxic to aquatic organisms. Ammonia dissolved in water is formed as a result of anaerobic decomposition of nitrogen-containing compounds from waste streams. Ammonium monitoring is extremely important in determining the quality of drinking water [1] and in open water, in places of wastewater discharge [24].

The increased content of ammonium indicates the deterioration of the sanitary condition of the water. The increase in concentrations is due to the inflow of domestic wastewater, nitrogen and organic fertilizers into groundwater. The content of ammonium in high concentrations in drinking water negatively affects the human body. Blood pressure may rise, there are various disorders of the liver and kidneys. The toxic effect of ammonium depends on the concentration and duration of consumption of contaminated drinking water, it increases with increasing pH. Short-term consumption of water with a concentration of ammonium salts in the range of 75–360 mg/kg causes an increase in blood pressure. Under conditions of prolonged exposure to drinking water with high levels of ammonium, there is a decrease in calcium in the body, changes in blood pH and weight loss [25].

Electrodes and methods for measuring fluoride, nitrate and ammonium.

Recently, a significant amount of research in the field of electrochemical research is aimed at developing more practical electrodes and biosensors for measuring fluoride, nitrate, ammonium and other elements in the aquatic environment using new technologies and various research methods. The main research directions are aimed at using ISE for the analysis of nitrate in natural objects: in water [9, 17, 19, 23, 24], in different environments [26–28]; application of voltammetric methods of analysis [16, 18, 21, 29, 30]; the use of the element copper in nitrate sensors [18, 20, 22, 30–34]; composite graphite, glass-carbon, graphene electrodes, nanotubes and nanotechnologies for measuring nitrate [33, 35–40]; new sensors and methods for measuring ammonium and nitrate [41–44].

This is by no means a complete list of scientific studies aimed at the application of new technologies and technical means of measuring fluoride, nitrate and ammonium in various fields, but it confirms the current relevance of studying the effects of these chemical elements on human health and the environment.

To ensure control of the content of these chemical elements in water and in the environment, it is necessary to increase the reliability and accuracy of concentrations. Since the performance of electrochemical studies and determination of concentrations of chemical elements in water is quite relevant, so the task is to develop methods for the determination of fluoride ions, nitrate and ammonium in drinking water.

The purpose of the paper is to use a chronoionometric method of measuring concentrations, the principle of which is based on the use of direct potentiometry, to determine the content of fluorides, nitrates and ammonium in drinking water and to determine the metrological characteristics of accuracy.

APPLICATION OF THE CHRONOIONOMETRIC METHOD OF DETERMINATION OF CONCENTRATIONS

The method of chronoionometry is based on the principle of potentiometric analysis, according to which the force difference is measured. The essence of the method is to determine the activity 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 electromotive force (EMF) of the electrode system on the concentrations of ions.

The process of measuring potentials by chronoionometry in the analytical system "Analyzer SCP" is performed as follows: during the determination using an electrolyzer with a sample solution, which is installed on a magnetic stirrer, immersed in the solution electrodes (indicator ion-selective and comparative silver chloride), with constant solution at a speed of 4 KHz read the value of the measurement of potentials in the measurement cycle with a duration of one second for a given period of time T [2]. 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 the value of the potential E_i is determined. The obtained values of $E(t)$ in real time in the form of chronopotentiograms are displayed, 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.

The algorithm of the chronoionometry method 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 concentrations by the method of multiple additives [2].

MEASUREMENT OF FLUORINE, NITRATE AND AMMONIUM CONCENTRATIONS

Let us determine the relative errors of measuring the concentrations of chemical elements of fluoride, nitrate and ammonium ions in model solutions by the method of chronoionometry.

Fluoride. To measure the concentrations of fluorine ions by chronoionometry, electrochemical parameters of potential measurement (Table 1) and ion-selective electrodes are used: measuring electrode ELIS-131F [5] and comparative silver chloride electrode with double electrolytic key filled with 2 M HCl electrolyte.

Step 1. Determine the constant potentials of calibration solutions of fluoride:

- 1 calibration solution: 10^{-5} M NaF (0, 401 $\mu\text{g}/\text{cm}^3$) + 2 ml BROIS_F
- 2 calibration solution: 10^{-1} M NaF (4008 $\mu\text{g}/\text{cm}^3$) + 2 ml BROIS_F

BROIS_F is a buffer solution for regulating the total ionic strength: take a sample of 58.5 g NaCl + 15.0 g CH₃COOH + 102.0 g CH₃COONa · 3H₂O, transfer to a volumetric flask with a capacity of 1 dm³, to half filled with distilled water, dissolve and bring to the mark with distilled water.

Construct a calibration graph at two points in the fluorine measurement range (Fig. 1), which shows the determination of the constant potential of the model solution of 10^{-3} M NaF.

Step 2. In a model solution of 10 ml of 10^{-5} M NaF + 2 ml of BROIS_F ($C_F = 0.19 \text{ mg}/\text{dm}^3$) measure the fluoride potential $E_{\text{izm}} = -302.0 \text{ mV}$.

Table 1. *Electrochemical parameters of fluoride measurement*

Ion	Concentration range, $\mu\text{g}/\text{cm}^3$	Interval potential, mV	Duration measurement, s
F ⁻	0,19–1900	from -500 to -200	60–180

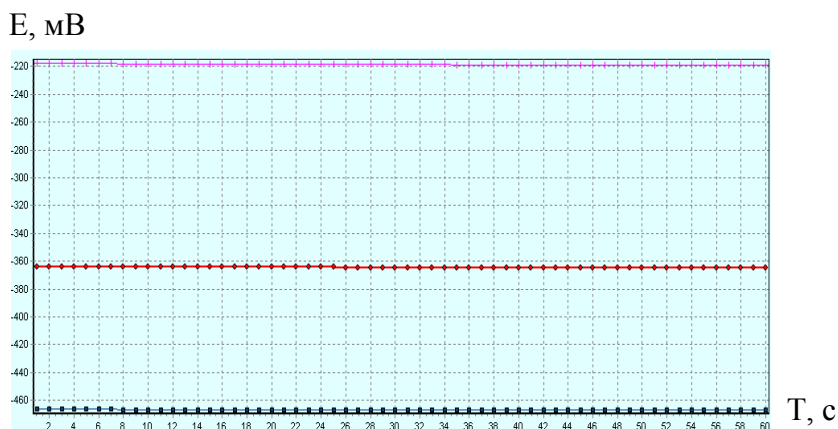


Fig. 1. Chronopotentiograms of potentials of calibration solutions of fluoride ions

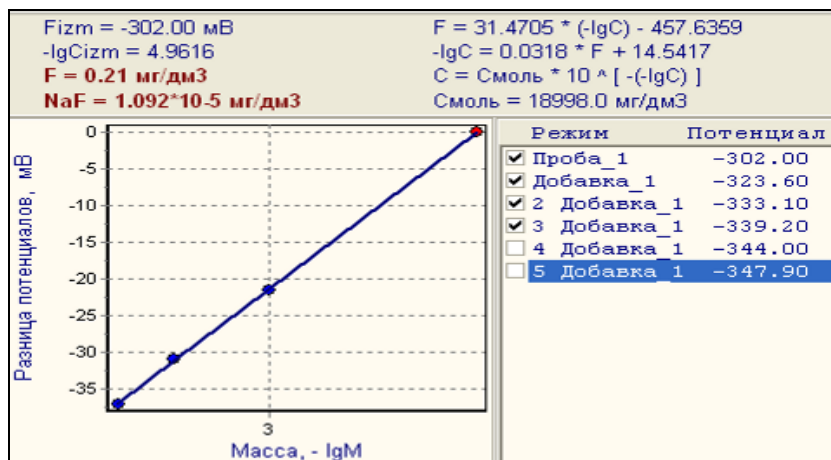


Fig 2. Determination of fluoride ion concentrations

Step 3. Determine the mass of the additive $M_F = 19.0 \mu\text{g}$ of a solution of 10^{-3} M NaF.

Step 4. Measure the constant potential of the fluoride ion in the sample solution for the three additives (Fig. 2).

Step 5. Calculate the concentration of fluoride ions in the model solution and plot the electrode characteristics for the three additives (Fig. 3).

Result. For the model solution of $1.0 \cdot 10^{-5}$ NaF mol/dm³ ($C_F = 0.19 \text{ mg/dm}^3$), according to the calculations (Fig. 2), the concentration of fluorine in the solution is $1.092 \cdot 10^{-5}$ NaF mol/dm³ ($C_F = 0.21 \text{ mg/dm}^3$), with a relative error of 9.2 %.

Nitrate. To measure nitrate concentrations by chronoionometry, electrochemical parameters of potential measurement (Table 2) and ion-selective electrodes are used: measuring electrode ELIS-121NO3 [5] and comparative silver chloride electrode with double electrolytic key filled with 2 M HCl electrolyte.

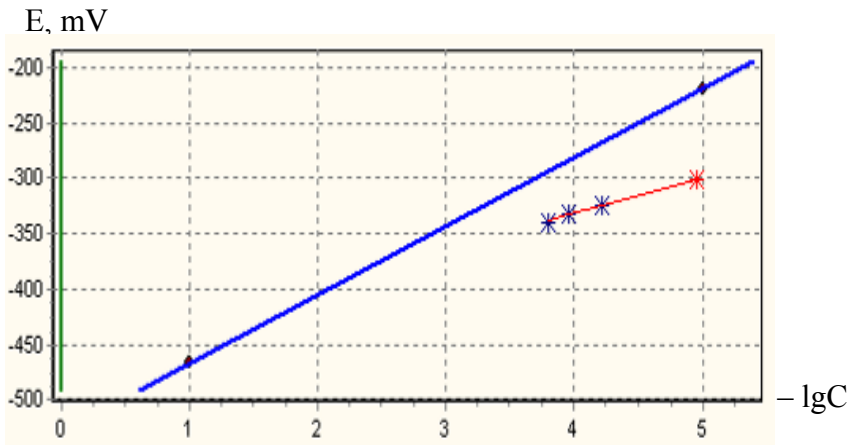


Fig 3. Electrode characteristic of fluoride ion measurement

Table 2. Electrochemical parameters of nitrate measurement

Ion	Concentration range, $\mu\text{g}/\text{cm}^3$	Interval potential, mV	Duration measurement, s
NO_3^-	0.62–6200	from 320 to 460	60–180

Step 1. Determine the constant potentials of calibration solutions of nitrates:

- 1 calibration solution: 10^{-5} M KNO_3 ($0.62 \mu\text{g}/\text{cm}^3$)
- 2 calibration solution: 10^{-1} M KNO_3 ($6200 \mu\text{g}/\text{cm}^3$)

Construct a calibration graph at two points in the range of measurement of nitrates (Fig. 4).

Step 2. In a model solution of 10^{-5} M KNO_3 ($C_{\text{NO}_3} = 0.62 \text{ mg}/\text{dm}^3$) measure the potential of nitrates $E_{\text{izm}} = +444.40 \text{ mV}$.

Step 3. Determine the weight of the additive $M_{\text{NO}_3} = 62.0 \mu\text{g}$ of a solution of 10^{-3} M KNO_3 .

Step 4. Measure the constant values of the potential of nitrates in the sample solution for the three additives (Fig. 5).

Step 5. Calculate the concentration of nitrates in the model solution and plot the electrode characteristics for the three additives (Fig. 6).

Result. For the model solution of $1.0 \cdot 10^{-5} \text{ KNO}_3 \text{ mol}/\text{dm}^3$ ($C_{\text{NO}_3} = 0.62 \text{ mg}/\text{dm}^3$), according to the calculations (Fig. 5), the concentration of nitrates in the solution is $0.994 \cdot 10^{-5} \text{ KNO}_3 \text{ mol}/\text{dm}^3$ ($C_{\text{NO}_3} = 0.62 \text{ mg}/\text{dm}^3$), with a relative error of 0.56 %.

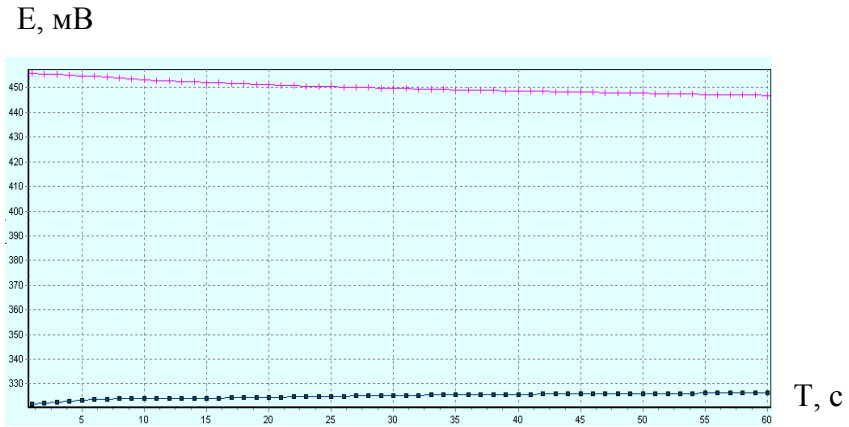


Fig. 4. Chronopotentiograms of potentials of calibration solutions of nitrates

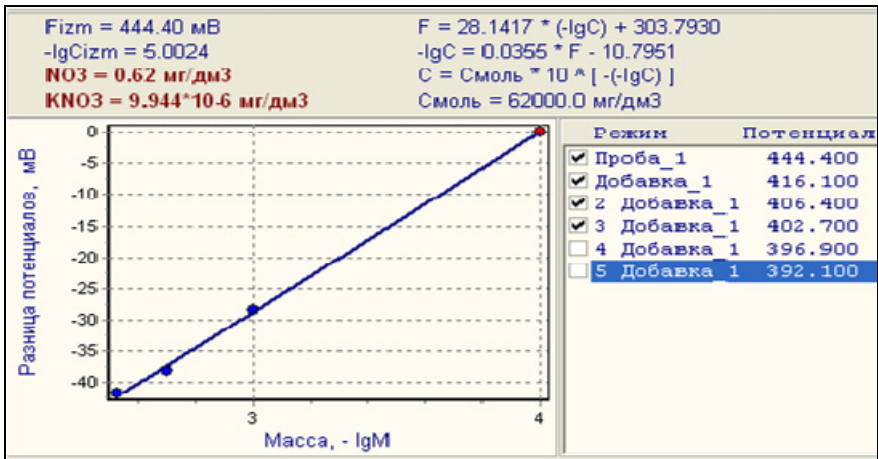


Fig. 5. Determination of nitrate ion concentrations

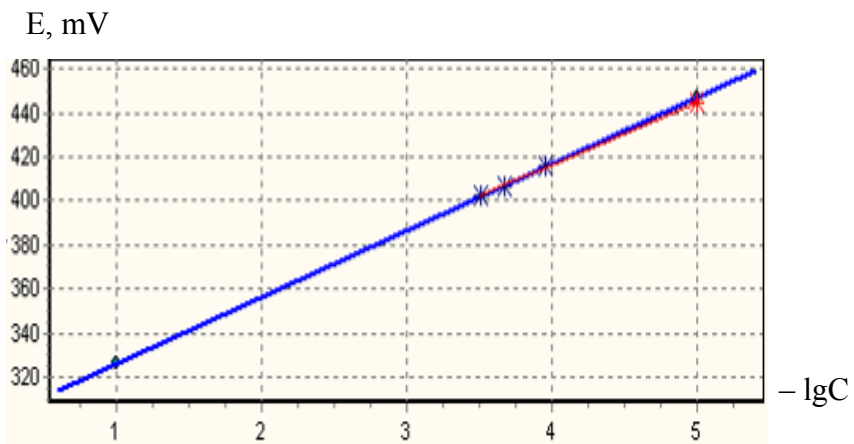


Fig. 6. Electrode characteristic of nitrate measurement

Table 3. Electrochemical parameters of ammonium measurement

Ion	Concentration range, $\mu\text{g}/\text{cm}^3$	Interval potential, mV	Duration measurement, s
NH_4^+	0.18–1810	from 300 to 550	60–180

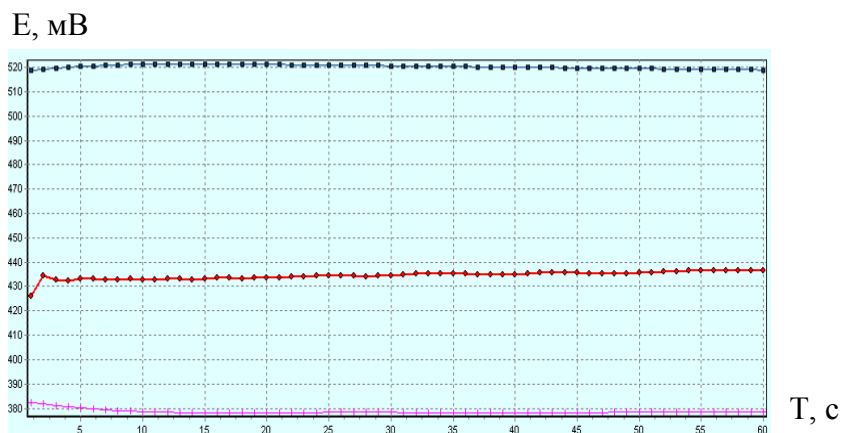


Fig. 7. Chronopotentiograms of potentials of calibration solutions of ammonium

Ammonium. To measure ammonium concentrations by chronoionometry, electrochemical parameters of potential measurement (Table 3) and ion-selective electrodes are used: measuring electrode ELIS-121NH₄ [5] and comparative silver chloride electrode with double electrolytic key filled with 2 M HCl electrolyte.

Step 1. Determine the constant potentials of the calibration solutions of ammonium:

- 1 calibration solution: 10^{-5} M NH_4Cl ($0.18 \mu\text{g}/\text{cm}^3$) + 2 ml $\text{BROIS}_{\text{NH}_4}$
- 2 calibration solution: 10^{-1} M NH_4Cl ($1810 \mu\text{g}/\text{cm}^3$) + 2 ml $\text{BROIS}_{\text{NH}_4}$

$\text{BROIS}_{\text{NH}_4}$ — buffer solution to regulate the total ionic strength: take a portion of 110.99 g of CaCl_2 (pre-dried), transfer to a volumetric flask with a capacity of 1 dm^3 , half filled with distilled water, dissolve and bring to the mark distilled water.

A calibration graph is constructed at two points in the fluoride measurement range (Fig. 7), which shows the determination of the constant potential of the model solution of 10^{-2} M NH_4Cl .

Step 2. In a model solution of 10 ml of 10^{-2} M NH_4Cl + 2 ml of $\text{BROIS}_{\text{NH}_4}$ ($C_{\text{NH}_4} = 181 \text{ mg}/\text{dm}^3$) measure the ammonium potential $E_{\text{izm}} = 408.7 \text{ mV}$.

Step 3. Determine the weight of the additive $M_{\text{NH}_4} = 1810 \mu\text{g}$ of a solution of 10^{-1} M NH_4Cl .

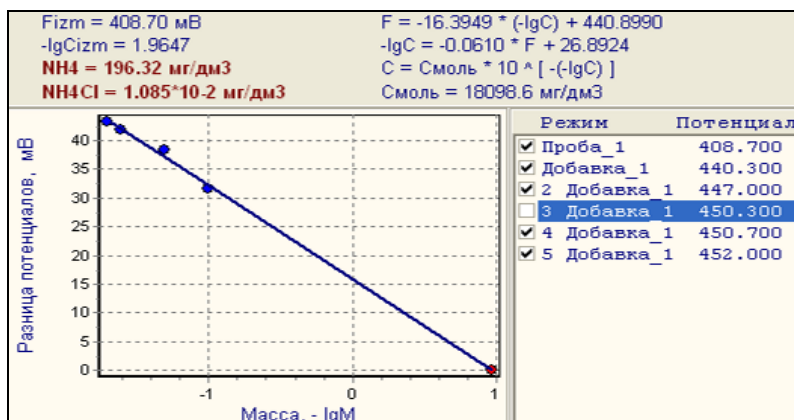


Fig 8. Determination of ammonium ion concentrations

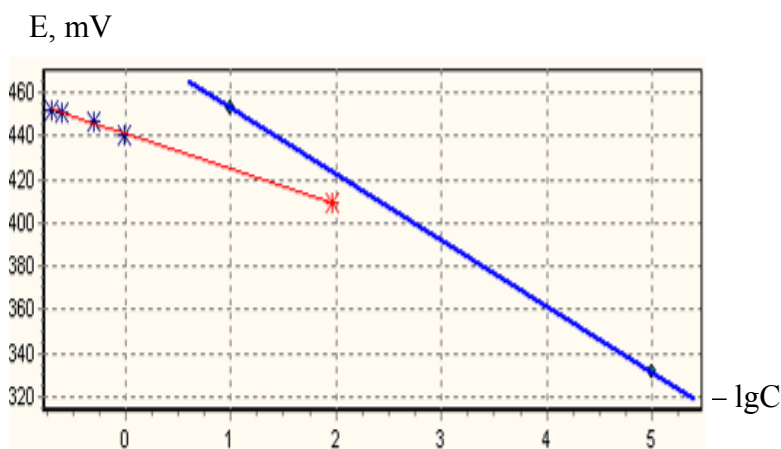


Fig 9. Electrode characteristic of ammonium measurement

Step 4. Perform measurements of constant indicators of the ammonium potential in the sample solution for five additives, additive 3 is not taken into account (Fig. 8).

Step 5. Calculate the concentration of ammonium in the model solution and plot the electrode characteristics for the four additives (Fig. 9).

Result. For the model solution of $1.0 \cdot 10^{-2}$ NH₄Cl mol/dm³ (C_{NH₄} = 181 mg/dm³), according to the calculations (Fig. 8), the concentration of ammonium in the solution is $1.085 \cdot 10^{-2}$ NH₄Cl mol/dm³ (C_{NH₄} = 196.32 mg/dm³), with a relative error of 8.5%.

FEATURES OF ALGORITHM IMPLEMENTATION IN INFORMATION TECHNOLOGY

The principles of implementation of the algorithm of the chronoionometry method in the analytical system "Analyzer SCP" are described [2]. Let us dwell on the developed module "Determination of ion concentrations" (Fig. 2, Fig. 5, Fig. 8). The window of this module provides the parameters for calculating the concentrations of the ion of the element, the graph of the potential difference from the logarithm of the mass for the selected potentials of the sample and additives involved in the calculation.

The parameters for calculating the concentrations given in the module window (Fig. 8) have the following values:

F_{izm} — the potential of ammonium (E_{NH_4}) in the model solution, mV;

$-\lg C_{izm}$ — activity of solution NH_4Cl (pNH_4);

NH_4 — concentration of ions NH_4^+ in the model solution of NH_4Cl , mg/dm^3

NH_4Cl — concentration of model solution, mol/dm^3 ;

F — record of the linear equation of the calibration graph of the dependence of the potential F on the concentrations ($-\lg C$) of solution NH_4Cl (the coefficient of linear dependence at ($-\lg C$) has the value of the slope of the electrode characteristic, its absolute value should not exceed the passport values for a particular ISE) ;

$-\lg C$ — inverse linear equation of the calibration graph of the dependence of the concentrations ($-\lg C$) of the solution NH_4Cl on the potential F;

C — mathematical formula for calculating ion concentration;

C_{mol} — the value of the molar concentration of ions ammonium, mg/dm^3 .

Note: If several potentials are involved in the calculation, the average value of these potentials is taken into account when plotting.

To determine the concentrations of fluoride F^- , nitrate NO_3^- , ammonium NH_4^+ ions in water, methods for measuring chemical elements, confirmed by patents were developed: a device for determining the concentration by CHI [47], a method for determining nitrate ions in aqueous solutions [48], fluoride ions [49] and ammonium ions [50]. 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 [51].

The effectiveness of the chronoionometric method for determining the concentrations of fluoride, nitrates and ammonium in drinking water has been proven by comparison with the characteristics of analytical systems developed in other countries.

ANALYSIS OF ACCURACY OF MEASUREMENT OF CONCENTRATIONS BY THE CHRONIONOMETRY METHOD

Assessment of safety and quality of drinking water is carried out according to epidemic safety indicators, sanitary-chemical and radiation indicators, according to hygienic standards [1]. 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 at values that are below the maximum permissible concentrations (MPC). This is due to the fact that the concentrations of chemical elements should not exceed the standardized values of sanitary and toxicological indicators of safety and quality of drinking water, which is an important factor in the prevention of human diseases.

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

The results of the studies to determine the measurement of concentrations of chemical elements fluorine, nitrate and ammonium in water show that the relative errors are in the range from 0.56 % to 9.2 %, which is less than the normalized relative measurement error.

Table 4. Comparison of measuring ranges of "Analyzer SCP" and sanitary-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⁾		
Fluoride (F) ⁴⁾	0.7	1.5	0.7	0.7	0.7	0.7–1.2	0.2–6000
Nitrate (NO ₃)	50	50	10	50	5	-	0.2–6000
Ammonium (NH ₄)	-	-	-	0,5	-	-	0,2–6000

Notes:

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

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 for the person of chemical substances polluting water depending on their toxicity, limiting sign of harm and the ability to cause adverse long-term effects).

Prospects for the development of the method and information technology

The main principle of practical implementation of chronoionometry methods in toxicological research is reliable measurement of fluoride ions, nitrates, ammonium, as well as potassium, sodium and calcium in determining the safety of drinking water and human environment to prevent the most common diseases, the use of the results of analysis of biological fluids in digital medicine, as well as the study of opportunities to improve methods for diagnosing the human condition using the results of analysis of ions of toxic chemical elements and compounds.

The developed method of chronoionometric measurement of ions in drinking water and in various environmental objects can be extended to other inorganic and organic compounds, for which there are ion-selective electrodes and verified methods of their measurement.

The proposed information technology architecture for determining the content of chemical elements in polluted water allows to develop an advanced highly sensitive analytical system based on the use of the device "Analyzer SCP" [52] and new electrochemical research methods that will improve environmental quality monitoring and assess human health risks drinking water.

Further development of information technology will be carried out using modern Internet technologies and a device for express electrochemical analysis of toxic elements, determining the principles of construction of a device for express electrochemical analysis of toxic elements in drinking water and the development of a set of programs for forecasting the risks of disease in terms of consumption of contaminated drinking water.

CONCLUSIONS

In the conditions of intensive anthropogenic impact of heavy metals on the ecosystem it is very important to carry out ecological monitoring of environmental objects, to assess risks for people in case of consumption of polluted drinking water. The possibility of such an analysis provides the use of IT, which is based on the developed algorithm for measuring the mass concentration of chemical elements in drinking and natural water.

The developed analytical system "Analyzer SCP" allows to determine the concentrations of 14 toxic elements in drinking water and in the environment (Hg, As, Pb, Cd, Cu, Zn, Sn, Ni, Co, Se, Mn, I, Cr, Fe) by inversion chronopotentiometry and six elements (K, Na, Ca, NH₄, NO₃, F) by chronoionometry, a total of 20 chemical elements. By chronoionometry, using ion-selective electrodes, you can determine the content of 11 more anions and cations (Ag⁺, Cl⁻, Br⁻, Li⁺, Ba²⁺, ClO₄⁻, CO₃²⁻, CN⁻, CNS⁻, S²⁻, TI⁺), these chemical elements can be added in the future to the analytical system "Analyzer SCP" with the appropriate development of methods for measuring the concentrations and presence of ion-selective electrodes.

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МЕТОД ХРОНОІОНОМЕТРИЧНОГО ВИЗНАЧЕННЯ КОНЦЕНТРАЦІЙ ФТОРУ, НІТРАТІВ, АМОНІЮ У ПИТНІЙ ВОДІ

Вступ. Використання методу хроноіонометрії та іон-селективних електродів дає можливість швидко визначити концентрації хімічних елементів, що дає змогу оцінити якість питної води та екологічний стан об'єктів довкілля.

Мета статті — застосувати розроблений метод хроноіонометрії для вимірювання концентрацій фтору, нітратів, амонію у питній воді та оцінити точність вимірювання концентрацій.

Методи. Хроноіонометричний метод хімічного аналізу використовує принципи прямої потенціометрії для вимірювання концентрацій хімічних елементів.

Результати. Розроблено способи виявлення концентрацій фтору, нітратів, амонію у питній воді та проведено тестування в модельних водних розчинах з використанням приладу інверсійної хронопотенціометрії «Аналізатор ІХП», які свідчать про відповідність похибок вимірювання концентрацій метрологічним нормативним значенням.

Висновки. Удосконалено аналітичну систему «Аналізатор ІХП» для визначення концентрації 20 хімічних елементів (Hg, As, Pb, Cd, Cu, Zn, Sn, Ni, Co, Se, Mn, I, Cr, Fe, K, Na, Ca, F, NO₃, NH₄) у водних розчинах методами інверсійної хронопотенціометрії та методом хроноіонометрії, що цілком достатньо для екологічного оцінювання якості питної води та об'єктів навколишнього середовища. Застосування нового методу хроноіонометрії значно розширює функціональні можливості приладу інверсійної хронопотенціометрії, підвищує надійність та точність вимірювання концентрацій хімічних елементів.

Ключові слова: метод хроноіонометрії, концентрація, фтор, нітрати, амоній, селективні електроди, інверсійна хронопотенціометрія, питна вода.