

Determination of Homologues Anion Surfactants in Technical Preparations Using a Multisensor System and HPLC

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Received April 30, 2016; in final form, May 24, 2016

Abstract—New potentiometric solid-contact sensors with polyvinyl chloride membranes based on compounds of alkyl sulfates with cationic complexes copper(II)–organic reagent are proposed for the determination of synthetic anionic surfactants (ASs). Multisensor systems are developed for the quantitative determination of ASs in raw technical preparations (alkylbenzene sulfonates, alkyl sulfates, and sodium cocosulfate).

Keywords: surfactants, potentiometric sensors, technical preparations, multisensor systems, HPLC

DOI: 10.1134/S1061934816110083

Synthetic surfactants form one of the most widespread classes of chemical compounds. Anion surfactants possess washing, moistening, emulsifying, dispersing, and other properties, are, therefore, widely used in different industries, and belong to environment pollutants.

The use of surfactants in different branches of human activity attracts special attention to the development and sophistication of methods for the control of their quality and concentrations in various objects. Different versions of spectroscopic, electrochemical, chromatographic, and electrophoretic methods are known for the determination of synthetic surfactants in waters, synthetic detergents and cleaning agents, medicines, foodstuffs, biological fluids, air, soils, and sedimentary deposits [1, 2].

Potentiometry with wide variety of sensors developed by state-of-the-art technologies offers a promising tool of chemical analysis for the rapid and highly sensitive determination of surfactants in various samples (raw technical preparations, household chemicals, cosmetics and hygienic preparations, medicinal substances, etc.).

State-of-the-art electrochemical sensor technologies represent a promising direction in the separate determination of different organic and inorganic compounds and the creation of multisensor systems of the electronic tongue type. The main types of sensors and sensing materials used in multisensor systems of the electronic tongue type and also the operation principles and main directions of their application were considered in the works [3–10]. The multisensor approach opens up a possibility of gaining information about the composition and concentrations of individ-

ual components in complex samples. Multisensor systems are developed and used for the analysis of foodstuffs and drinks, medicines, biological fluids, model solutions, and industrial process solutions.

Raw materials for the production household chemicals, technical preparations, sewages of industrial enterprises, and other samples are systems of complex composition, including mixtures of surfactants of different nature. This explains the urgency of the problem of the efficient separation of surfactants followed by the determination of concentrations of individual surfactants, both in industrial and environmental samples.

This work is devoted to the separate determination of homologues ASs (alkyl sulfates, alkylbenzene sulfonates) in technical preparations (sulfonol, sodium lauryl sulfate, sodium cocosulfate) using an array of AS sensors based on copper (II)–organic reagent–alkyl sulfate compounds and HPLC.

EXPERIMENTAL

We used sodium alkyl sulfates with the concentration of the main substance 98–99% (Table 1). Stock solutions of surfactants with concentrations 1×10^{-2} – 1×10^{-3} M were prepared by dissolving precisely weighed portions of preparations in distilled water; working 1×10^{-3} – 1×10^{-7} (1×10^{-6}) M solutions were obtained by consecutive dilutions. We investigated cationic surfactants (dodecylpyridinium chloride, **DDP** and cetylpyridinium chloride, **CPC**) and technical surfactant-containing preparations (sulfonol, sodium lauryl sulfate, and sodium cocosulfate).

Table 1. Names and formulas of the studied ASs and technical preparations

Substance	Formula	Designation
Sodium decyl sulfate	$C_{10}H_{21}OSO_3Na$	DS
Sodium undecyl sulfate	$C_{11}H_{23}OSO_3Na$	UDS
Sodium dodecyl sulfate	$C_{12}H_{25}OSO_3Na$	DDS
Sodium tridecyl sulfate	$C_{13}H_{27}OSO_3Na$	TDS
Sodium tetradecyl sulfate	$C_{14}H_{29}OSO_3Na$	TTDS
Sodium hexadecyl sulfate	$C_{16}H_{33}OSO_3Na$	HDS
Sodium alkylbenzene sulfonates (ZAO "Plant of Organic Products," Dzerzhinsk, OAO "Kirishineft'orgsin- tezh," Kirishi, Russia)	$C_nH_{2n+1}C_6H_4SO_3Na, n = 10-16$	—
Sodium lauryl sulfate Empicol LXV/N (Huntsman Corp.)	$ROSO_3Na$ $R = C_nH_{2n+1}, n = 12, 14$	—
Sodium cocosulfate Mackol CAS-100N (Rhodia)	$ROSO_3Na$	—

We studied solid-contact potentiometric sensors with plasticized membranes and graphite as an electron conductor. The sensor membranes were fabricated from polyvinyl chloride (PVC) of the S-70 brand, tetrahydrofuran and dibutyl phthalate (DBP). The PVC : DBP ratio was 1 : 3, $c_{ionophore} = 1-2\%$. The ionophores were as follows:

- ion pairs of alkyl sulfates with alkylpyridinium;
- compounds of alkyl sulfates with cationic complexes of copper (II) and some *N*-donor chelating organic reagents (pyridine, **Pyr**; 1,10-phenanthroline, **Phen**; 2,2'-dipyridyl, **Dip**) and also with *N,N'*-bis-(salicylidene) ethylene diamine (**Salen**) and a cationic CPC additive.

Plasticized polyvinyl chloride membranes and solid-contact sensors were fabricated as described in [11–13].

The compositions of ionophores were determined by the data of elemental and thermogravimetric analyses, UV and IR spectrometry. The ionophores are thermally resistant substances (stable to about 100–120°C) and do not contain substantial amounts of water in the crystal lattices.

Potentiometric measurements were performed with an Ekspert-001-3(0.1) potentiometer with an error of ± 1 mV at $20 \pm 3^\circ C$; the reference electrode was a standard silver–silver chloride EVL-1MZ electrode. To accelerate the achievement of the steady-state value of the potential, solutions were stirred with a magnetic stirrer. The selectivity of the studied membranes was estimated by the method of spiked solutions.

The accuracy of the determination of ASs was controlled by HPLC. For the chromatographic determination of homologues sodium alkyl sulfates and sodium alkylbenzene sulfonates in technical prepara-

tions, we used a chromatographic Agilent 1260 HPLC system, consisting of a high-pressure pump, a device for automatic sample injection with a 100- μ L loop, a thermostat ($t_{col} = 30^\circ C$), and a vacuum degasser. Homologous sodium alkylbenzene sulfonates were determined with a diode array detector adjusted to the wavelength $\lambda = 254$ nm [14] and homologues sodium alkyl sulfates, with a light scattering detector. The collection and processing of the chromatographic data were carried out using the ChemStation software for the LC 3D system (Rev.B.04.03). The mixtures of substances were separated on an AcclaimTM Surfactant Plus column (Thermo Scientific, United States) of the diameter 4.6 mm and length 150 mm, packed with an adsorbent with a particle size of 5 μ m. A sample of a preparation was obtained by dissolution in the mixture H_2O-CH_3OH (50 : 50). The concentrations of substances in the test solutions were no more than 15 mg/mL. To reduce the time of analysis, we used linear bigradient elution: mobile phase A, aqueous 0.1 M CH_3COONH_4 buffer solution (pH 5.0–5.2) and mobile phase B, acetonitrile.

Selectivity coefficients were determined by the method of spiked solutions.

Anionic surfactants in model solutions and the main concentrations in raw technical preparations were determined by potentiometric precipitation titration using surfactant sensors; the titrant was a 1×10^{-2} – 1×10^{-4} M solution of CPC. The titration endpoint was determined graphically, by the difference method, and also by the Gran method [15].

The multisensor approach was used for the separate determination of homologues ASs in aqueous solutions and technical samples. Analytical signals from a sensor array were processed by the method of artificial neural networks (ANN) (Statistica 6.1). The criterion

of the optimum architecture of the network was the minimization of the error. The input signals were processed using the known approach based on the distribution of input data over three sets. Calibration (training) mixtures were used to train the neural network; validation mixtures were used for the choice of networks with the optimum architecture, control of training activity, prevention of network retraining; and test mixtures allowed the estimation of the reliability of the obtained calibration model and the control of quality of predictions. The responses of sensors (input data) were randomly divided into training, validation, and test sets in the ratio 2 : 1 : 1. The input data for training and testing the network were values of sensors potentials, and the output data were values of concentrations (pc). The sensor responses were measured not less than three times for each mixture. The starting data were the average values of sensor potentials of the array. Neural networks with the architecture of a three-layer perceptron (TLP) were trained using the algorithm of the back propagation of errors and the method of conjugate gradients. Preliminary data processing was performed by methods of mean correction and normalization. A correlation between the sensor signals was controlled using principal component analysis (Unscrambler 4.0), which allowed visualization of the similarities and distinctions in the behavior of sensors. The correlation was judged by the mutual arrangement of points in a score plot constructed for 21 sensors with different compositions of membranes in quinary mixtures.

RESULTS AND DISCUSSION

We studied sensors based on ion pairs of alkylpyridinium alkyl sulfates and cationic copper(II) complexes with Salen (Phen, Dip). Sensors exhibited sensitivity to homologues sodium alkyl sulfates in a wide concentration range (Fig. 1). The main electrochemical properties of solid-contact AS sensors based on different ionophores in solutions of homologues sodium alkyl sulfates (dodecyl-, three-, tetra-, hexadecyl sulfate) are summarized in Table 2.

The slopes of the electrode functions of sensors approached the Nernstian slope for singly charged ions (48–66 mV/ pc). The deviation of electrode functions from linearity was due to the solubility of active membrane components at concentrations lower than 1×10^{-7} (4×10^{-7}) M and micelle formation at concentrations higher than 1×10^{-2} (5×10^{-4}) M. The lowest limit of detection (1×10^{-7} M) was observed for sensors based on $[\text{Cu}(\text{Phen})_2]\text{DDS}_2$ and $[\text{Cu}(\text{Dip})_2]\text{DDS}_2$ in DDS, TDS, TTDS, and HDS solutions.

The emergence of an electrode potential at the membrane–test solution interface is due to the dissociation of ion exchangers, ion pairs of dodecyl sulfate with cationic Cu(II) complexes of Salen (Phen, Dip)

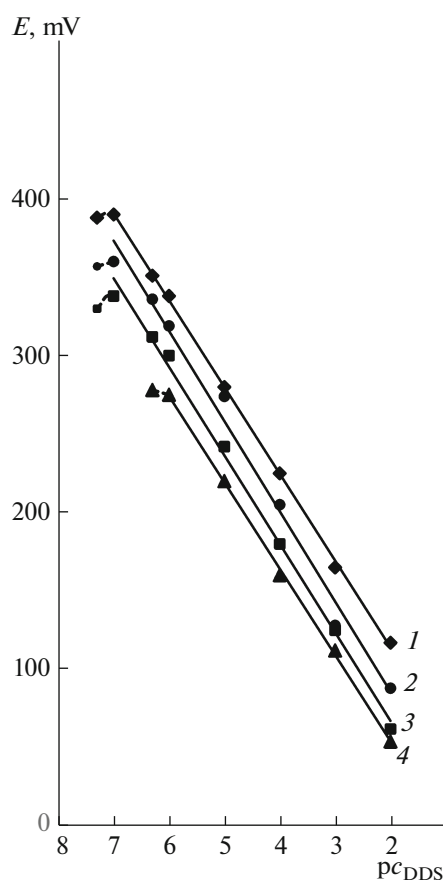


Fig. 1. Electrode functions of sensors based on (1) $[\text{Cu}(\text{Pyr})_4]\text{DDS}_2$, (2) $[\text{Cu}(\text{Dip})_2]\text{DDS}_2$, (3) $[\text{Cu}(\text{Phen})_2]\text{DDS}_2$, and (4) CP–DDS in DDS solutions. $c_{\text{ionophore}} = 1\%$.

in the membrane phase and ion-exchange processes at the membrane–solution interface.

Stable complexes of Cu(II) with *N*-donor chelating organic reagents in the inner sphere favored the formation of strong and poorly soluble ion pairs with homologues sodium alkyl sulfates, which, in turn, ensured the high ion-exchange capacity of membrane compositions on their basis.

The effect of interfering anions on the results of potentiometric determination of DDS for sensors was close to the Hofmeister lyotropic series of anions and pointed to the ion-exchange mechanism of sensor response. Based on selectivity coefficients, we found that the studied sensors ensured the determination of alkyl sulfates in the presence of acetates, salicylates, nonionic surfactant, and inorganic anions (Cl^- , F^- , I^- , Br^- , NO_3^- , NO_2^- , ClO_4^- , SCN^- , CO_3^{2-} , SO_4^{2-} , PO_4^{3-}). The AS sensors did not possess selectivity to the basic alkylsulfate anion but exhibited sensitivity to other homologues sodium alkyl sulfates ($K_{\text{pot}} \rightarrow 1$).

Determination of homologues anionic surfactants in model mixtures. The developed sensors were used in

Table 2. Electrochemical characteristics of sensors based on different ionophores in solutions of homologues sodium alkyl sulfates ($c_{\text{ionophore}} = 1\%$, $n = 3$, $P = 0.95$)

Ionophore	Surfactant solution	$E = f(c)$; linearity range, M	$\alpha \pm \Delta\alpha$, mV/pc	c_{min} , M
CP–DDS	DS	$1 \times 10^{-6} - 1 \times 10^{-2}$	55 ± 1	9×10^{-7}
	DDS	$1 \times 10^{-6} - 1 \times 10^{-2}$	55 ± 2	9×10^{-7}
	TDS	$1 \times 10^{-6} - 5 \times 10^{-3}$	61 ± 1	9×10^{-7}
	TTDS	$1 \times 10^{-6} - 1 \times 10^{-3}$	63 ± 2	9×10^{-7}
	HDS	$1 \times 10^{-6} - 5 \times 10^{-4}$	66 ± 2	9×10^{-7}
[Cu(Pyr) ₄]DDS ₂	DS	$5 \times 10^{-7} - 1 \times 10^{-2}$	51 ± 2	4×10^{-7}
	DDS	$3 \times 10^{-7} - 1 \times 10^{-2}$	55 ± 2	2×10^{-7}
	TDS	$3 \times 10^{-7} - 5 \times 10^{-3}$	56 ± 1	2×10^{-7}
	TTDS	$3 \times 10^{-7} - 1 \times 10^{-3}$	58 ± 2	2×10^{-7}
	HDS	$3 \times 10^{-7} - 5 \times 10^{-4}$	64 ± 2	2×10^{-7}
[Cu(Dip) ₂]DDS ₂	DS	$5 \times 10^{-7} - 1 \times 10^{-2}$	49 ± 1	4×10^{-7}
	DDS	$2 \times 10^{-7} - 1 \times 10^{-2}$	57 ± 1	1×10^{-7}
	TDS	$2 \times 10^{-7} - 5 \times 10^{-3}$	56 ± 1	1×10^{-7}
	TTDS	$2 \times 10^{-7} - 1 \times 10^{-3}$	61 ± 1	1×10^{-7}
	HDS	$2 \times 10^{-7} - 5 \times 10^{-4}$	64 ± 2	1×10^{-7}
[Cu(Phen) ₂]DDS ₂	DS	$5 \times 10^{-7} - 1 \times 10^{-2}$	48 ± 1	4×10^{-7}
	DDS	$2 \times 10^{-7} - 1 \times 10^{-2}$	57 ± 2	1×10^{-7}
	TDS	$2 \times 10^{-7} - 5 \times 10^{-3}$	59 ± 1	1×10^{-7}
	TTDS	$2 \times 10^{-7} - 1 \times 10^{-3}$	62 ± 2	1×10^{-7}
	HDS	$2 \times 10^{-7} - 5 \times 10^{-4}$	64 ± 1	1×10^{-7}
[CuSalen] with a CP additive	DS	$8 \times 10^{-7} - 1 \times 10^{-2}$	50 ± 1	7×10^{-7}
	DDS	$4 \times 10^{-7} - 1 \times 10^{-2}$	58 ± 2	3×10^{-7}
	TDS	$5 \times 10^{-7} - 5 \times 10^{-3}$	59 ± 1	4×10^{-7}
	TTDS	$5 \times 10^{-7} - 1 \times 10^{-3}$	62 ± 2	4×10^{-7}
	HDS	$5 \times 10^{-7} - 5 \times 10^{-4}$	65 ± 1	4×10^{-7}

the multisensor analysis of multicomponent mixtures of sodium alkyl sulfates. Arrays of sensors with membranes of different compositions, containing compounds of homologues sodium alkyl sulfates (DS, DDS, TDS, TTDS, HDS) with CP [Cu(Pyr)₄]²⁺, [Cu(Phen)₂]²⁺, [Cu(Dip)₂]²⁺, and also a sensor based on [CuSalen] with a CP additive were created (the maximum number of sensors was 21).

The assessment of a correlation between the sensor signals showed that the greatest difference in sensitivity was observed for sensors based on Cu(II)–Pyr (Dip, Phen)–DS(DDS, TTDS, HDS), and [CuSalen] with a cationic surfactant additive (only 12–13 sensors). The contribution of the first three components to the total explained dispersion was 85% (PC1, 31%; PC2, 30%; PC3, 24%; PC4, 11%; PC5, 4%).

Signals from other sensors were correlated, i.e., exhibited similar sensitivity. On the other hand, it was found that, with an increase in the number of sensors in the array (starting from 10 and above), the average relative error (D) of the determination changed insignificantly (by no more than 1.7%); therefore, in the further experiments we used arrays consisting of 10–12 sensors.

The predictive ability of ANN was estimated depending on the number and concentration range of calibration mixtures, method of preparation of the starting data, and architecture of the network. To train ANN, we used solutions of homologues sodium alkyl sulfates with concentrations 1×10^{-6} , 1×10^{-5} , and 1×10^{-4} M (taking into account all ratios of mixture components at these concentration). The accuracy of

the determination was controlled by the added–found method using reference model mixtures (Fig. 2). The smallest average relative error of the determination of homologues sodium alkyl sulfates (2.3% DS, 1.3% DDS, 4.4% TDS, 2.2% TTDS, and 2.0% HDS) was

obtained using a three-layer perceptron. To check the predictive ability of ANN, were prepared model mixtures with component concentrations outside the concentration range for training the multisensor system, i.e., $> 1 \times 10^{-4}$ M (Fig. 2). It was found that the average

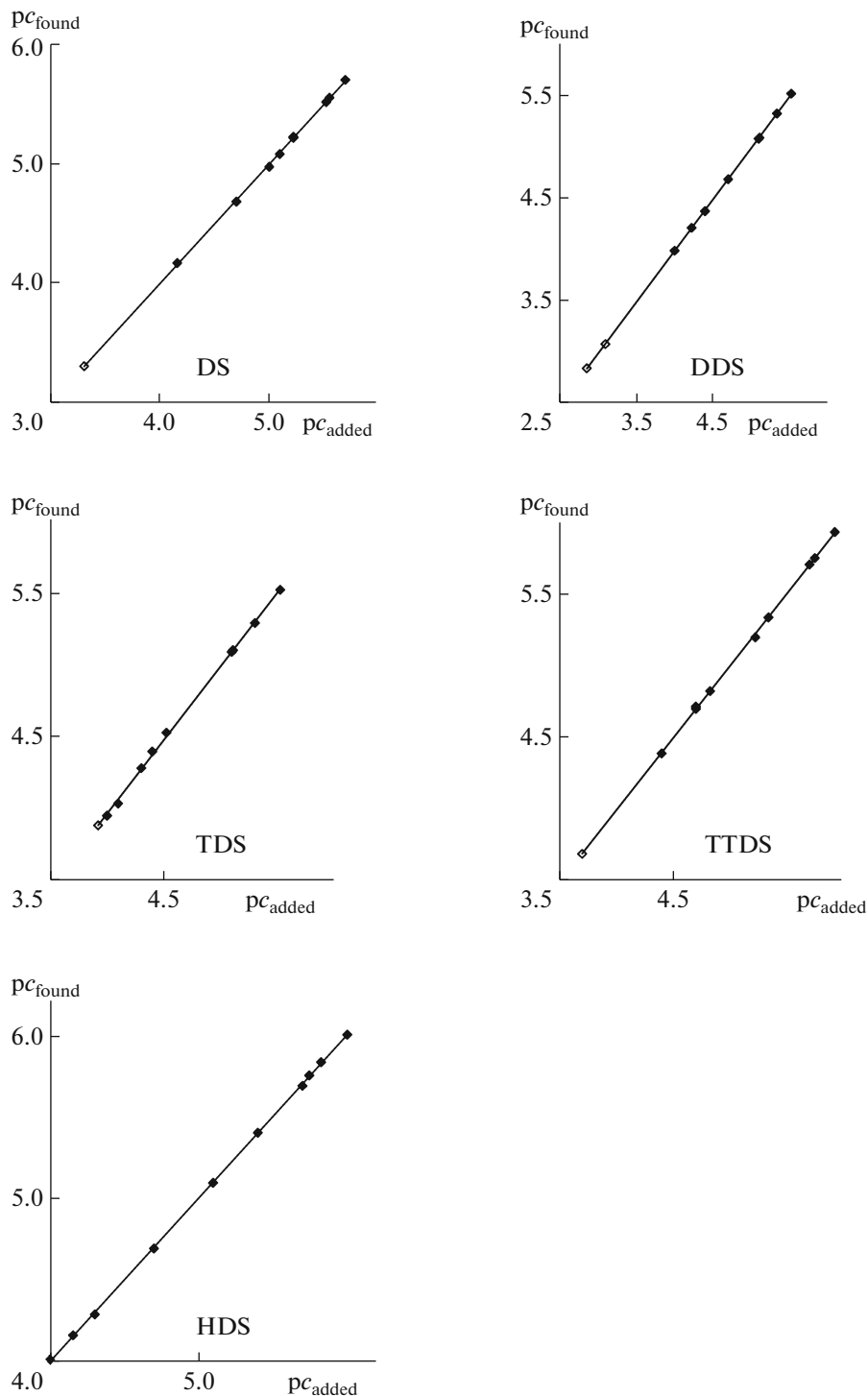


Fig. 2. Determination of sodium alkyl sulfates in quinary model mixtures. (◆) Homologue concentration outside the concentration range for training ANN ($> 1 \times 10^{-4}$ M).

Table 3. Results* of the simultaneous determination of sodium alkyl sulfates in quinary model mixtures by the ANN method (TP 10-13-5) (combined set) ($n = 3$, $P = 0.95$)

Mixture	c_{DS} , M	D , %	c_{UDS} , M	D , %	c_{DDS} , M	D , %	c_{TDS} , M	D , %	c_{TTDS} , M	D , %
1	3×10^{-5}	5.5	1×10^{-8}	1.9	1×10^{-8}	6.8	1×10^{-8}	2.5	1×10^{-8}	1.0
	$(3.17 \pm 0.08) \times 10^{-5}$		$(9.81 \pm 0.17) \times 10^{-9}$		$(1.07 \pm 0.02) \times 10^{-8}$		$(9.75 \pm 0.16) \times 10^{-9}$		$(9.90 \pm 0.08) \times 10^{-9}$	
2	7×10^{-6}	2.6	1×10^{-8}	4.4	5×10^{-5}	0.9	1×10^{-8}	9.2	1×10^{-8}	3.1
	$(7.18 \pm 0.14) \times 10^{-6}$		$(1.04 \pm 0.01) \times 10^{-8}$		$(4.96 \pm 0.03) \times 10^{-5}$		$(9.08 \pm 0.23) \times 10^{-9}$		$(9.69 \pm 0.10) \times 10^{-9}$	
3	8×10^{-5}	2.1	1×10^{-8}	1.2	3×10^{-6}	2.3	9×10^{-6}	2.0	1×10^{-8}	3.2
	$(7.83 \pm 0.13) \times 10^{-5}$		$(1.01 \pm 0.01) \times 10^{-8}$		$(2.93 \pm 0.03) \times 10^{-6}$		$(8.82 \pm 0.20) \times 10^{-6}$		$(1.03 \pm 0.02) \times 10^{-8}$	
4	4×10^{-6}	3.1	1×10^{-8}	5.6	5×10^{-5}	1.8	2×10^{-6}	1.7	4×10^{-5}	3.6
	$(4.13 \pm 0.10) \times 10^{-6}$		$(9.44 \pm 0.15) \times 10^{-9}$		$(5.09 \pm 0.07) \times 10^{-5}$		$(1.97 \pm 0.03) \times 10^{-6}$		$(4.14 \pm 0.06) \times 10^{-5}$	
5	5×10^{-5}	5.2	1×10^{-8}	0.1	5×10^{-6}	2.9	9×10^{-5}	1.9	1×10^{-8}	9.8
	$(4.74 \pm 0.09) \times 10^{-5}$		$(9.99 \pm 0.13) \times 10^{-9}$		$(4.85 \pm 0.05) \times 10^{-6}$		$(8.83 \pm 0.14) \times 10^{-5}$		$(1.10 \pm 0.03) \times 10^{-8}$	
6	6×10^{-5}	0.1	1×10^{-8}	3.2	7×10^{-6}	4.0	3×10^{-5}	3.3	4×10^{-5}	2.3
	$(5.99 \pm 0.10) \times 10^{-5}$		$(9.68 \pm 0.13) \times 10^{-9}$		$(7.28 \pm 0.09) \times 10^{-6}$		$(3.10 \pm 0.06) \times 10^{-5}$		$(4.09 \pm 0.04) \times 10^{-5}$	

* For each mixture component, the added (upper) and found ($c \pm \Delta c$) (lower) concentrations, M, are given.

relative error of the determination of such concentrations of homologues did not exceed 15%. In addition, to estimate the predictive ability of the multisensor system in the analysis of samples of unknown composition and reference mixtures containing a smaller number of components than the mixtures used to train ANN, it was expedient to use sets of mixtures consisting of different numbers of homologues (DS, UDS, DDS, TDS, TTDS).

Because of the impossibility of using the preprocessing of input data for components with "zero" concentrations (absence of component), in this case we used homologue concentration below the limit of its detection with the sensor array (1×10^{-8} M). Therefore, the check of predictive ability was reduced to the calibration of ANN with quinary mixtures including conditionally zero component concentrations (Table 3). It was found that the average relative error of the determination of homologues in such mixtures was 3.1% for DS, 2.7% for UDS, 3.1% for DDS, 3.4% for TDS, and 3.8% for TTDS. The optimum architecture of the neural network was TP 10-13-5.

Therefore, multisensor analysis ensures the prediction of concentrations of homologues sodium alkyl sulfates above and below the calibration range. The results of training a neural network in a multicomponent mixture were used in the subsequent analyses of reference mixtures containing equal or smaller numbers of components and in the determination of the homologues distribution of ASs in raw technical preparations.

Determination of the homologous distribution of ASs in raw technical preparations (sulfonol, sodium lauryl sulfate, sodium cocosulfate). Sulfonol samples represented mixtures of sodium alkylbenzene sulfonates with the lengths of hydrocarbon chains $C_{10}H_{21}$ – $C_{14}H_{29}$, i.e., a quinary mixture of homologous AS, sodium lauryl sulfate and sodium cocosulfate, a mixture of homologues alkyl sulfates with the lengths of hydrocarbon radicals $C_{12}H_{25}$ and $C_{14}H_{29}$ (a binary mixture of homologues). The concentration of the main substance in technical preparations was determined beforehand. Titration curves for some samples of technical preparations are presented in Fig. 3 and the results of determination of the main substance, in Table 4. To train the neural network, we used pure quinary mixtures of homologues sodium alkyl sulfates with the lengths of hydrocarbon radicals $C_{10}H_{21}$ – $C_{14}H_{29}$ (DS, UDS, DDS, TDS, TTDS) and $C_{10}H_{21}$ – $C_{16}H_{33}$ (DS, DDS, TDS, TTDS, HDS). The optimum architecture of the neural network was TP 10-13-5.

The results of determination of the homologous distribution of anionic surfactants in the studied sulfonol samples using a multisensor AS–HPLC system are summarized in Table 5. For sulfonol no. 3, the homologue with the length of hydrocarbon radical $C_{10}H_{21}$ was not found, and this was confirmed by the results of HPLC. Similarly, homologues with the lengths of

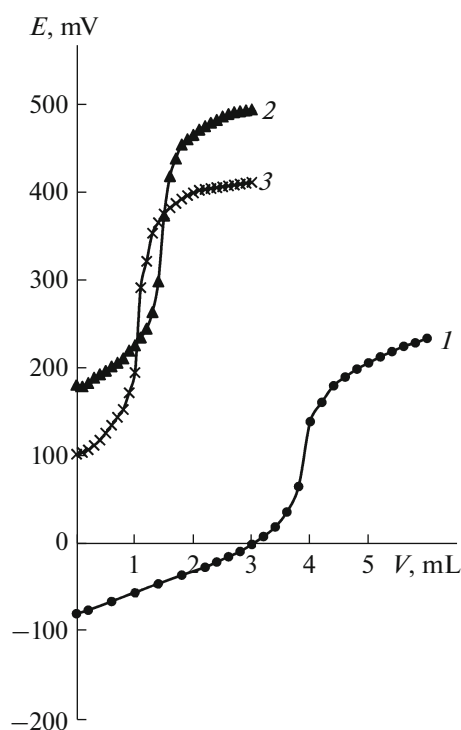


Fig. 3. Curve of titration of technical preparations of (1) sulfonol, (2) sodium lauryl sulfate, and (3) sodium cocosulfate. Ionophores: (1) [CuSalen], (2) [Cu(Phen)₂]DDS₂, (3) [Cu(Dip)₂]DDS₂. *V* of sodium alkyl sulfate solution, mL: 1, 2; 2, 3; 1. Titrant, 1×10^{-3} M CP.

hydrocarbon radicals $C_{10}H_{21}$, $C_{11}H_{23}$, and $C_{13}H_{27}$ were not found in the composition of sodium lauryl sulfate, and the concentrations of homologues $C_{12}H_{25}$ and $C_{14}H_{29}$ (77.7 and 13.9%) found by two different methods correlated with each other. In addition, the $C_{16}H_{33}$ homologue (1.7%) was found in the sample of sodium lauryl sulfate. A comparison of the results obtained with a multisensor HPLC system by the *F*- and *t*-tests showed the absence a systematic error.

Table 4. Determination ($\bar{\omega} \pm \Delta\omega$, wt %) of main substance concentration in technical preparations (concentration of ASs declared $\geq 80\%$; ionophores: [Cu(Phen)₂]DDS₂; $n = 3$, $P = 0.95$)

Sample	Potentiometric titration	HPLC
Sulfonol no. 1	96.1 ± 0.9	95.6 ± 0.6
Sulfonol no. 2	82.0 ± 1.2	82.5 ± 0.4
Sulfonol no. 3	94.2 ± 1.4	93.8 ± 0.5
Sodium lauryl sulfate	92.6 ± 1.4	93.2 ± 0.4
Sodium cocosulfate	90.8 ± 1.4	91.5 ± 0.7

Table 5. Determination of the homologous distribution of sodium alkyl sulfates in sulfonol samples ($n = 3$, $P = 0.95$)

Method	Homologous distribution, %			
	C ₁₀ H ₂₁	C ₁₁ H ₂₃	C ₁₂ H ₂₅	C ₁₃ H ₂₇
	Sulfonol no. 1			
Multisensor AS system	10.94 ± 0.32	30.68 ± 0.11	31.88 ± 0.26	22.39 ± 0.26
HPLC	10.74 ± 0.10	30.63 ± 0.10	31.71 ± 0.10	22.52 ± 0.09
	Sulfonol no. 2			
Multisensor AS system	10.69 ± 0.27	25.48 ± 0.37	27.46 ± 0.45	19.26 ± 0.40
HPLC	10.51 ± 0.09	25.25 ± 0.10	27.75 ± 0.11	18.99 ± 0.13
	Sulfonol no. 3			
Multisensor AS system	–	17.83 ± 0.25	65.24 ± 0.56	6.56 ± 0.15
HPLC	–	17.92 ± 0.10	64.85 ± 0.11	5.90 ± 0.10

* * *

Thus, the architecture of ANN was optimized by neural network modeling for the processing of the data of multisensor systems in quinary mixtures of sodium alkyl sulfates. A possibility of the practical use of multisensor systems including sensors with the optimum electroanalytical characteristics for the determination of homologous distribution in multicomponent model mixtures and technical raw preparations was shown.

ACKNOWLEDGMENTS

This work was performed within the State Contract of the Ministry of Education and Science of the Russian Federation in the Sphere of Scientific Activity (Basic Component) no. 4.1212.2014/k, code “Fluorofor.”

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Translated by E. Rykova