An Adaptive Spectroellipsometric Technology for the Diagnosis of Water Ecosystems

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Abstract— Ellipsometry is an optical technique that uses the change in the state of polarization of light upon reflection and refraction for the in-situ and real-time characterization of surfaces, interfaces, liquid solutions in the hydrochemical investigations. Spectroellipsometry methods are used for the undestroying investigation of chemical and physical characteristics of liquid solutions. The diagnostics of liquids gives possibility to assess the concentration of chemicals dissolved and weighed in the liquid as well as to determine the spots of pollutants on the water surface.

A compact measuring — information multi-channel spectroellipsometric system for monitoring the quality of aquatic environment, that is based on the combined use of spectroellipsometry and training, classification, and identification algorithms is described. This system is differed from modern analogues by the use of a new and very promising method of ellipsometric measurements, an original element base of polarization optics and a complex mathematical approach to estimating the quality of a water object subjected to anthropogenic influence. The spectroellipsometric system can be used in different fields where the water quality should be estimated or the presence of a particular set of chemical elements should be revealed.

1. INTRODUCTION

Problem of the aquatic environment operative diagnostics is arisen practically in many human base including agriculture, medicine, industry and service. The development of these anthropogenic processes poses the problem of water pollution control and synthesizing monitoring system for water quality assessment in active regime.

Pollutant sources can have different structures and classes. Therefore, monitoring system is to be multi-purpose and mobile. It can be realized with the use of spectroellipsometric technology that gives possibility to have the spectrums with the sensitivity of 0.01% [1, 2].

The creation of multi-channel polarization optical instrumentation and use of spectroellipsometric technology are very important for the real-time ecological control of aquatic environment. It should be mentioned that efficient solution of this multi-parametric problem greatly depends on the precision and simplicity of ellipsometric devices. A technology of combined use of spectroellipsometry and algorithms of optical spectrums identification and recognition allows the creation of a standard integral complex of instrumental, algorithmic, modular and software tools for the collection and processing of data on the aquatic environment quality with forecasting and decision — making functions [2–4].

This paper describes new version of spectroellipsometric system that develops and realizes the functions of contaminant identification for multi-component solutions. It is realized by means of combined use of cluster analysis and algorithms for inverse task solution.

2. METHODOLOGY

Spectroellipsometric expert system for the aquatic environment diagnostics (SESAED) consists of measuring subsystem and software. The system's structure includes a compact multi-channel spectroellipsometer (MCS), information interface with computer (IIC), software (STW), and extending database (EDB). The STW realizes a number of algorithms to process data fluxes from the MCS and provides the service functions of visualization and control of measurements. The EDB consists of sets of standard spectral images of aquatic environments represented by points in the multi-dimensional vector space of indicators, pre-calculated on the basis of learning samples.

The principle behind the SESAED is based on fixing changes in light flux the MCS and digitizing them in IIC. Further processing of these data to make them more efficient is determined by STW with algorithms capable of recognizing spectral images. The degree of adaptability of the recognition procedure is determined by the level of accumulated knowledge about intensity fluctuations and the polarizing properties of light reflected from the water surface or dispersed and refracted within the water environment. The STW enables, in case of uncertain identification of spectral images, to make an expert decision based on the visual analysis of a spectral image. This procedure is realized in dialog mode with the SESAED and, if a decision is made, the operator can fix it in the database in the form of a standard for subsequent appearances of similar spectral images.

Spectroellipsometric measurements deliver spectrums that are considered as spectral images of water solutions. Space of spectral images is formed during the learning procedure realized in laboratory conditions when spectral images and chemical analysis are performed at the same time. Identification procedure to recognize spectral image of water solution is carried out with the use of the EDB where spectrums and their derivatives are storage during learning procedure. Standard of the EDB item is given in Table 1.

Table 1: Structure of standard spectral image of water solution. Notation: A_1 is the square occupied by spectral curve, A_2 is the maximal value of spectral curve, A_3 is the minimal value of spectral curve, A_4 is the distance between wavelengths with minimal and maximal values of spectral curve, respectively; A_5 is the maximal derivative of spectral curve; A_6 is the maximal value of second derivative of spectral curve; A_7 is the number of spectral curve maximums; A_8 is the average value of spectral curve; A_9 is the wavelength corresponded to average value of spectral curve; B is the chemical element concentration.

Etalon number	A_1	A_2	A_3	A_4	A_5	A_6	A_7	A_8	A_9	B
1	A_{11}	A_{21}	A_{31}	A_{41}	A_{51}	A_{61}	A_{71}	A_{81}	A_{91}	B_1
...										
n	A_{1n}	A_{2n}	A_{3n}	A_{4n}	A_{5n}	A_{6n}	A_{7n}	A_{8n}	A_{9n}	B_n

An identification of spectral image for unknown water solution is realized by means of comparison his vector — identifier with elements of the EDB. Depending from used optical device spectral image of water solution can be represented by one or two vector-identifiers calculated with the use of rule described in Table 2. Final identification is realized by means of search in the EDB of vector — identifiers which are minimal distance from considered vector-identifier $Q = \{X_1, \ldots, X_n\}$ of given water solution. Distance between vector-identifiers is calculated with the use of the following formula:

$$\delta = \min_n \rho\left(Q - Q_n\right) = \frac{1}{2n} \min_i \left[\sum_{j=1}^{n} \left| X_j - A_j^i \right| + \sqrt{\sum_{j=1}^{n} \left(X_j - A_j^i \right)^2} \right] \tag{1}$$

Use of (1) gives better result in comparison with the application of other known criteria of closeness between spectral curves. That is why in this case there is minimal risk to miss the situation with dangerous pollution of water reservoir. In common case, usually the following methods are used:

•*Cluster analysis.* In this case two types of clusters are formed for $\cos\Delta$ and $\tan\Psi$ where Δ and Ψ are ellipsometric angles corresponding to complex amplitude reflection coefficients for two different polarizations. Decision is made by weighted values (1) or independently for each polarization.

•*Algorithm of discrepancy between spectra.* It is assessed average distance between the ordinates for both spectra and spectrum of studied case and decision is made taking into account minimal value of this distance.

•A*lgorithm of discrepancy between etalon vectors.* In this case, decision is made taking into consideration of minimal δ.

•*Inverse task solution.* This algorithm is based on linear dependence of optical spectrum on the concentration of chemical elements in water solution. In this case, sub-definite system of linear algebraic equations is solved.

3. RESULTS

The SESAED was used in different laboratory and in-situ conditions. Table 2 shows example of vector-identifiers calculated for $CuSO_4$ 10% solution with use of Table 1 procedure. Table 3 gives experimental results which give possibility to compare above mention algorithms. Dependence of risk assessment as function of solution concentration is represented in Fig. 1. As it follows from these results risk to have high error under the solution identification is reduced when algorithm of Table 1 is used. We see that risk to have high error is growth with increase of chemical element concentration. It is caused that discrepancy between spectra is decreased with increase of chemicals concentration. In this case it is necessary to extend the database of spectral etalons.

Table 2: An example of the SESAEC database element.

Solution	Q	Vector-identifiers								
$CuSO_4$ (10%)	Q_Δ	21.6	0.17	0.1	143	0.67	0.12	2	0.16	0.21
	Q_Ψ	43.1	0.89	0.04	201	0.59	0.09	3	0.65	0.01

Table 3: Comparatively assessment of algorithms for recognition of spectral images of water solutions.

Object for study	Identification algorithm and its error (%)			
	Cluster analysis	Discrepancy between spectra	Discrepancy between vector-etalons with the use Equation (1)	Inverse task solution
$CuSO_4$	15	12	8	7
NaCl	17	11	7	5
$NaHCO_3$	16	10	5	5
NH_4OH	21	13	9	6
$ZnSO_4$	22	12	8	6
Potassium iodite	13	10	6	4
Na + Cu + Zn + Mn + glu	18	9	9	8
cose	23	11	5	5
Furaciline	14	10	4	4
Bifidumbacterium				

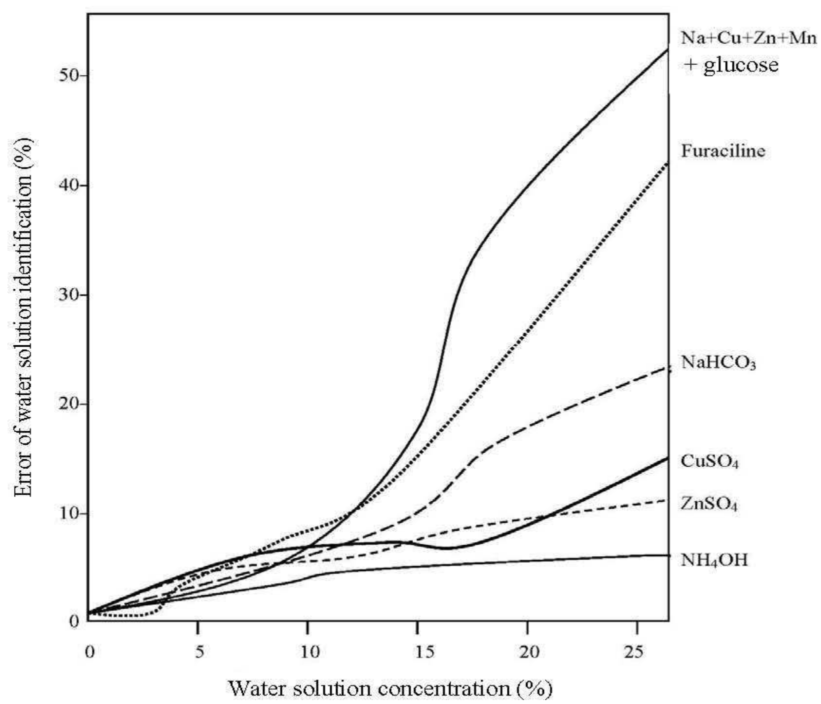

Figure 1: Dependence of spectral image identification on the solution concentration.

4. CONCLUSION

The main objective of work is to create in future the compact information systems for monitoring the quality of aquatic environment and to investigate their potential efficiency. These systems are based on the combined application of spectroellipsometry methods and algorithms of training, classification, and identification. The realization of this objective will require the combined use of engineering and algorithmic tools providing real — time measurements and data processing. The technology of combined use of spectroellipsometry and algorithms of detection and classification will allow the creation of an original system of instrumental, algorithmic, modular and software tools for the collection and processing of data on the aquatic environment with forecasting and decision-making functions. The theoretical part of the work will include the use of methods of polarization optics, mathematical statistics, the theory of pattern recognition and mathematical modeling.

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