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Analyzer of Liquid Chemical Substances

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Abstract:
The article describes the principles of analysis of pollutants in water by molecular absorption spectrometry. The spectrometer is used for analysis. Design and implementation of software for the evaluation of water analysis is part of the work. The software is designed with ease of use and retrieval of data. Analysis of water is mainly focused on nitrates. The detection is focused on determining levels of particular components, suitable algorithm recognizes the substance.

Anotace:
Článek popisuje principy analýzy znečišťujících látek ve vodě poímocí molekulární absorpční spektrometrie, pro analýzu se využívá spektrometr. Součástí práce je i návrh a implementace softwaru pro vyhodnocování analýzy vody. Software je navrženo tak, aby bylo možné analýzu a získávání dat provádět velmi jednoduše. Pozornost analyze vody je zaměřena především na dusičnany. Detekce se zaměřuje na stanovení koncentrací jednotlivých složek, látka se rozpoznává s využiítím vhodného algoritmu.

INTRODUCTION

Spectrophotometric measurements can be performed by two basic ways. Most currently used techniques are based on measurements under static conditions at equilibrium reaction (used at work). The conditions of quantitative course must be selected appropriately to achieve steady state, if the spectrophotometric response form the basis for its determination.
The method with the exchange of energy between radiation and the material under investigation (the spectrometric method) is used in the work. The energy exchange is the absorption or emission of radiation. Spectrometric methods are the basis of optical methods. Speed and reliability is an advantage of absorption spectroscopy. The methods allow analysis using a small amount of diagnosed substance, ones allows determination of low concentrations (tenths to hundredths of a percent).
As a rule, the paper should be divided into chapters, each with a heading, so that the reader can follow the logical development of the work. The introduction should state the objectives of the paper and give a review of earlier works. Theoretical considerations, mathematical derivations, technical details and experimental results should be left for posterior chapters.
Analytical use of molecular absorption spectrometry in the ultraviolet and visible regions are versatile in both organic and inorganic analysis. Information on the presence of typical groups in the molecule substances can be obtained from the qualitative analysis, using evaluation of obtained spectra of organic substances (qualitative assessment of the structure of matter). Radiation absorbs certain characteristic groups in the molecule (i.e. Chromophores) absorbed wavelength (absorption band location) related with their structure. Identification of the substance is not unique only by the resulting absorption spectra in the ultraviolet and visible region [1]. Analysis of the absorption spectra allows to deal the relations between the constitution of substances and their characteristic absorption. Position of the appropriate absorption spectrum is qualitative in nature, intensity of monitored absorption has quantitative character.

MEASUREMENT

The basis of measurement workplace was designed for analysis, the workplace consist from the source of photonic radiation as well as the spectrometer. The instruments are from the OceanOptics firm - Fig. 1. IOOBase32 software is used for controlling the operation of the analysis using the spectrometer. The software is used to collect data from the spectrometer and their transfer to the PC.

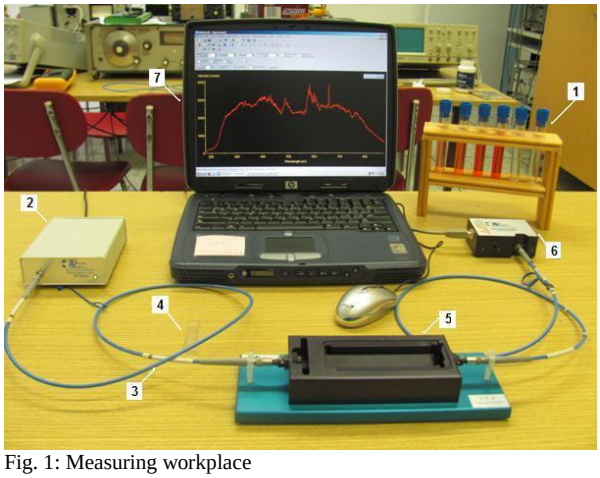

Fig. 1: Measuring workplace

USB2000 Spectrometer (company OceanOptics) formed the main part of the measuring system. The spectrometer operates on the principle of plug-and-play. The spectrometer can be connected to PC via USB cable only. The spectrometer is powered via USB, range of used wavelengths can be defined. Microspectrometer with 2048 CCD detector was used. Light passing through the cuvette is scattered in a grid from 200nm to 900nm. The spectrometer allows a choice of 14 grids and 6 slits for setting the most suitable parameters of the measurement system [2].

PC with OOIBase32 (company OceanOptics) was used to collect data from the spectrometer. The spectrometer evaluates the light passed through cuvette and sends data via USB cable to the PC. The program OOIBase32 allows you to display spectrum of received light according on the wavelength. The integration time for suitable reading of the spectrum can be set in the program, the program allows you to easily export data to excel form.

The cuvette was used to measure the absorbance of the solutions of various substances in the visible and near infrared range (from 350nm to 1000nm). The measured water sample was placed in a quartz glass cuvette with a volume of 4ml. The spectra of cuvettes from two types of glass was measured - Fig. 2. The broad spectrum source of the photonic radiation (from 200nm to 1100nm) (DT-Mini-2) was used, measurements were carried out in the wavelength range from 200nm to 900nm.

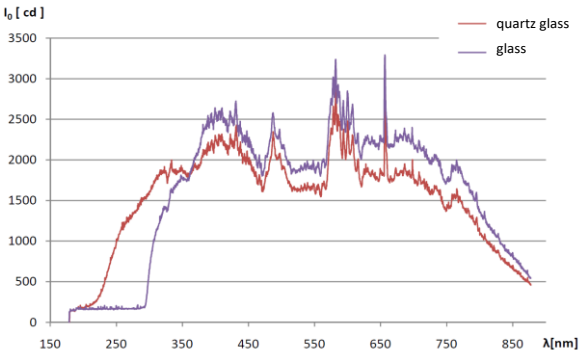

Fig. 2: The spectra of cuvettes from two types of glass

CONTROL OF ANALYSIS

The control software allows the creation of a user-friendly environment, which is used for the rapid control of analysis. The main focus is put on nitrate KNO_3 and $Ca(NO_3)_2$, software is able to analyzes the concentrations of $CuSO_4 \cdot 5(H_2O)$ and $KMnO_4$. The flow diagram of the program is on the Fig. 3. Matlab scripts („Analyzator vody 1.0“) were programmed to output data format (Excel). The flow diagram describes several operation steps, i.e. loading data, drawing graphs and calculation of the resulting concentration. An example of user environment is shown in Fig. 4.

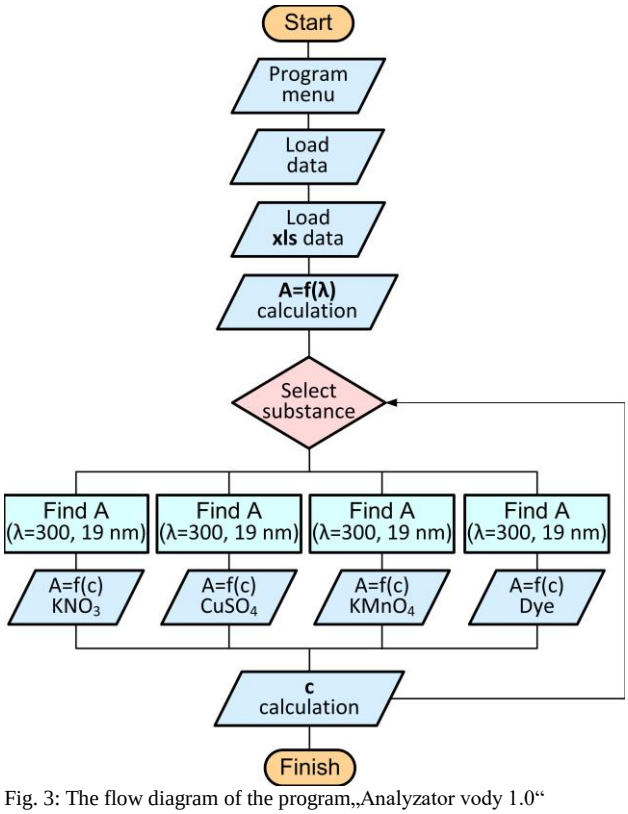

Fig. 3: The flow diagram of the program„Analyzator vody 1.0“

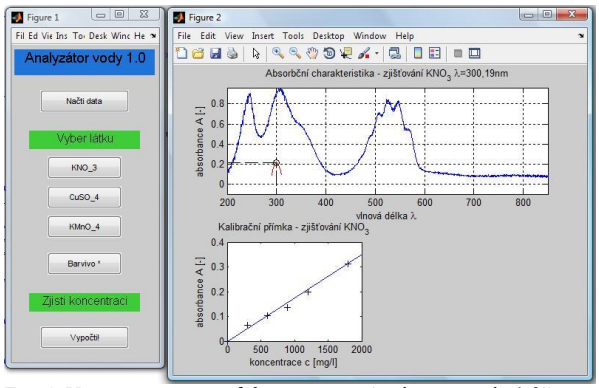

Fig. 4: User environment of the program „Analyzator vody 1.0“

REACHED RESULTS

Spectral characteristics were measured for several selected samples at various concentrations, an example is shown in Fig. 5. The concentrations of substances were calculated using the program „Analyzator vody 1.0“. Measurements are also performed by mixing two or three compounds. The analysis was implemented for a mixture of one, two and three substances. Deviations were calculated for the measured values using the theory of calculation errors. Method of determining the spectra of the individual substances in the mixture is shown in the work (Multicomponent analysis) method can also determine the concentrations of the individual components.

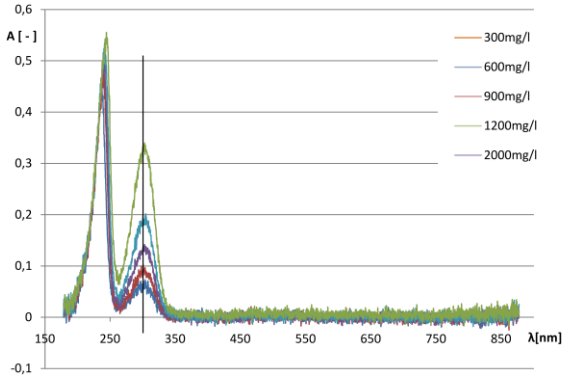

Fig. 5: The spectral absorption characteristics of KNO_3 in dependence on the wavelength

Spread spectrum of two substances can be obtained utilizing this method - for example, Fig. 6. Method, which is controlled by the program analyzer water 1.0 works on the principle of overlap of detection spectra. Principle of the method can be explained according to Fig. 6. According to the shape of the spectrum can be determined that the wavelength λ = 542.25 nm detect hypermanganate. Its spectrum at a concentration of 100 mg/l is drawn in red. If we subtract the spectrum from the spectrum alone hypermanganate mix, we get the spectrum itself nitrate, on the Fig. 6 is shown by dashed line. According to the calibration curve can be determined nitrate concentration.

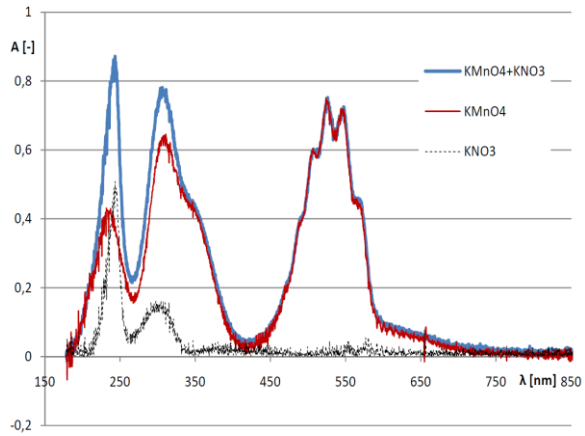

Fig. 6: A mixture of two substances

Spread spectrum of three substances can be obtained utilizing this method - for example, Fig. 7. Detection of three agents is more difficult. In the detection of three substances is to be expected overlapping spectra. In the figure is shown an example for a mixture of copper sulphate, hypermanganate and potassium nitrate. The way of detection of concentration is the same as for two substances. Several peaks of wavelengths can be determined from spectral lines. The increased absorbance value can be determined by the wavelength of a copper sulfate with λ = 783.36 nm. The concentration of a copper sulfate can be calculated from the absorbance value corresponding wavelength, etc.

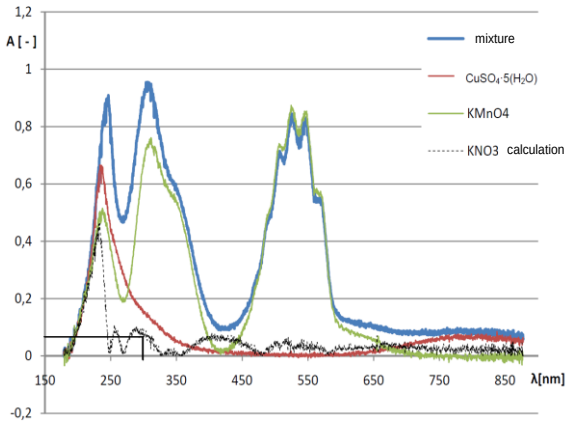

Fig. 7: A mixture of three substances

CONCLUSIONS

Graphic environment allows the user to resolve the presence of three substances in the solution. Proposed computing method enabled obtaining information about the types of substances in solution and its concentration. The proposed software enabled processing such data. The characteristic wavelength can be determined unambiguously from the graphs, the measured concentration of substances can be determined from these data obtained. The overlapping spectrum succeeded to analyze in a mixture of several substances. Software operates with output data from microspectrometer. The program includes a simple graphical environment for easy communication with the user. The program allows to read and store data from a microspectrometer, the program can calculate and plot the spectral absorption characteristics from the data.

ACKNOWLEDGEMENT

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