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Data Acquisition and Data Processing Challenges in Heavy Metal Measurements

J.M Dias Pereira, D.[1),2)], Salgado, R.[1),3)]

[1]LabIM, ESTSetúbal/IPS, Escola Superior de Tecnologia de Setúbal do Instituto Politécnico de Setúbal, Rua Vale de Chaves, Campus do IPS, Estefanilha, 2910-761 Setúbal, Portugal.
[2]Instituto de Telecomunicações, Av. Rovisco Pais, 1049-001, Lisboa, Portugal.
[3]REQUIMTE/CQFB, Chemistry Department, FCT, Universidade Nova de Lisboa, 2829-516 Caparica, Portugal.

*Corresponding author: dias.pereira@estsetubal.ips.pt; Tel: +351 265 790 000.

Abstract: *Water quality is a key factor to preserve human life quality, as well as, environmental and biological ecosystems. This paper highlights specific issues related with the acquisition and data processing of heavy metal measurement systems. Between the main challenges related with this kind of measurements, such as the ones related with the very low signal amplitudes to be measured, since very low concentrations, in the order of tens of p.p.b., of some heavy metals, can be very dangerous for human life and for ecosystems sustainability. Additional challenges, that are associated with online heavy metals measurements, are related with the capability to obtain accurate results using a low number of measurement points. The first part of the paper includes a survey of different measurement techniques that can be used for heavy metals' measurements, underlining the capabilities of voltammetric techniques. The main goal of the paper is a comparison of different data processing algorithms that can be used to improve heavy metal measurement accuracy when a segmented voltammetric voltage scan is performed to improve measurement celerity. Regarding data processing of the measurement data, B-Spline, Gaussian and artificial neural network based techniques are compared with traditional least mean square techniques based on polynomial curve fitting. The performance of each technique is evaluated in terms of the required number of measurement points, for a given root mean square deviation between curve fitted and experimental data. A brief comparison of the different techniques, in terms of insensitivity to errors caused by measurement data outliers, is also presented.*

Keywords: *Heavy metals, curve fitting methods, measurement data outliers, measurement accuracy, sensitivity and celerity.*

1. INTRODUCTION

Heavy metals (HM) are chemical elements with a specific gravity higher than 5, such as arsenic, cadmium, iron, lead and mercury, among others, and, some of them, can be very toxic for living organisms. In some cases, the toxic effect on the living organisms can be observed even when small concentrations of these elements are present in the environment. However, small amounts of HM can be an important micronutrient for many living organisms, as long as their concentrations is lower than specific thresholds. Above these thresholds, defined by international environmental organizations [EEA, EPA], HM are considered as pollutant and poisoned for the organisms. Acute and chronic diseases, caused by excessive HM concentrations, can affect the organisms depending on the exposure time and the concentration of these compounds. The organs more sensitive to this toxic effect are the lung, kidney and liver but effects on the blood composition and in the nervous system can be also observed due to the contact with HM in the environment.

Moreover, human activities can also contribute to increase the concentration of the HM and change the natural balance between the elements and compounds found in surface, groundwater and the coastal waters [MAN]. Thus, the measurement of concentration variability in the natural environment is a challenge for online monitoring HM concentrations that can affect the human life and the natural ecosystems. The water quality measurements are important to get information about retention time of the water, aquifers age, flows and recharge area and also in areas with irrigation or aquaculture systems. The monitoring plan and the environment measurements can help us to decide prohibitive areas and non-prohibitive areas for some specific activities due the contamination and pollution risk involved. The renewable of the estuary water in the aquaculture tanks should not have HM, or at least, they should be present in very small concentrations for bivalve aquaculture production (e.g oysters, bivalve in general and fishes).

Concerning HM measurement technologies, it is important to refer that sensors and micro devices (e.g. microelectrodes) had an extraordinary evolution in the last years and there exist promising solutions to perform heavy metals measurements based on micro-electromechanical-systems (MEMS) and bulk acoustic wave sensors (BAWS) [1,2]. Recent developments in MEMS and BAWS enabled the appearance of new solutions to measure a large number of chemical and biological quantities. Nevertheless, even if these measurement methods are very attractive in terms of hardware compactness, they exhibit several limitations, namely in terms of reproducibility, selectivity, cross-sensitivity and response time.

In the last years, the authors developed several research activities focusing their attention in water quality assessment systems. Low-cost solutions and prototypes for the measurement of water temperature, conductivity, dissolved oxygen, turbidity, pH and HM, have been presented and successfully tested in real measuring environments. This paper highlights specific measurement issues related with online HM measurements, in terms of measurement celerity and data processing.

Different curve fitting techniques of segmented voltammetric data are used to compare relative performance, in terms of the minimization of the number of measurement points for a given measurement accuracy, and in terms of the reduction of errors caused by measurement data outliers. There are a large number of curve fitting techniques that can be used to evaluate HM concentrations in water solutions [CF1-CF7]. However, comparative studies of the different techniques are not frequent and, above all, those comparative studies generally considers a continuous, and linear, voltammetric voltage scan and not a segmented voltammetric voltage scan, proposed by the authors to improve online HM measurement celerity.

The remaining part of this paper is organized as follows: section 2 includes a survey of several HM measurement methods underlining the main characteristics of electrochemical methods; section 3 focuses some specific issues related with the acquisition and data processing of HM measurement signals and section 4 performs a comparative analysis between the traditional polynomial, B-Spline, Gaussian and ANN based curve methods. The last part, section 5, is dedicated to conclusions.

5. CONCLUSIONS

This paper highlights specific issues related with the acquisition and data processing of heavy metal measurement signals. Concerning online measurements, electrochemical methods are presented as a powerful solution to perform heavy metals' measurements, and a segmented voltammetric voltage scanning technique, that improves measurement celerity, is used to evaluate curve fitting algorithms performance. Concerning curve fitting of measurement data, a comparative analysis between polynomial, Gaussian, B-Spline, and Artificial Neural Network curve fitting methods was performed. The performance of each method is evaluated in terms of the required number of measurement points, for a given root mean square deviation between curve fitted and experimental data, and in terms of sensitivity to interpolations errors caused by measurement data outliers. It was clearly shown, that the Gaussian curve fitting method outperforms the others methods that were used for comparative analysis. For example, the usage of the polynomial curve fitting method gives always a root mean square interpolation error higher than 10 % and the Gaussian curve fitting error, using the same number of measurement points, for curve fitting purposes, is always more than 10 times lower.

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