Título: APPLICATION OF CHEMOMETRIC METHODS TO WATER QUALITY STUDIES

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> QUIMICA ANALITICA

> ANALISIS MULTIVARIANTE

> QUIMICA DEL AGUA

> CONTROL DE LA CONTAMINACION DEL AGUA

El fichero de tesis no ha sido incorporado al sistema.

Resumen: Chemometric methods have been used to explore and analyze information regarding potable and waste water quality in this Thesis. The analyzed data were obtained from (a) drinking water disinfection processes, (b) wastewater treatment processes, (c) water sensorial analysis, and (d) laboratory experiments. This Thesis attempts to improve our knowledge regarding common water quality problems, such as the formation of trihalomethanes (THMs) disinfection by-products (in the Sant Joan Despi Drinking Water Treatment Plant of Barcelona, SJD-DWTP) and the main factors affecting their formation. Furthermore, the Thesis illustrates how to facilitate the monitoring of water quality in a Wastewater Treatment Plant of Girona town (WWTP) by applying chemometric methods. Further objectives of the Thesis include the development of a chemometric method for source apportionment, where drinking waters with different origins were blended (as it usually occurs inside the Barcelona drinking Water Distribution System, WDS) using measured ultraviolet absorbance and physicochemical parameters. This Thesis additionally considered the problem of water taste by developing models, where water taste is explained and predicted based on the mineral content of tap and bottled waters using panelists.

The chemometric methods, applied in this Thesis, have been applied to multi-parametric data matrices generated using different instrumental analyses techniques, such as laboratory UVVIS spectrophotometer, Gas Chromatograph with Electron Capture Detector (GC-ECD) and Inductively Coupled Plasma Optical Emission

Spectrometer (ICP-OES). Additionally, data was obtained by implementation of standard methods for estimation of different physicochemical parameters or by multi-parametric data extractions from the Laboratory Information Management System (LIMS). Data was also acquired from an automatic multi-parametric station for online monitoring and from carefully designed sensorial experiments.
In this Thesis, different linear projection based methods, such as Principal Component Analysis (PCA), Principal Component Regression (PCR) and Partial Least Squares regression method (PLS), have been used and shown as appropriate for handling data. Different linear regression methods have been compared to powerful nonlinear regression methods such as Kernel radial basis function Partial Least Squares (K-PLS) and Support vector machine regression (SVR) methods.
Among the most significant findings of this Thesis was the identification of a set of parameters, which are highly relevant for the trihalomethanes formation, such as water temperature, organic matter fractions and concentration, chlorine concentrations, turbidity, bromide/chloride ions concentrations, pumped underground water and carbon filters age. Chemometric models, with low prediction errors for all THMs species, have been developed at SJD-DWTP. The most important physicochemical parameters for panellist water taste liking were found to be: HCO3- , SO42-, Ca2+, and Mg2+ at moderate concentration of the overall mineralization and pH. Temporal variation with a different data frequency (daily, monthly and annual cycles) were observed in WWTP water quality and suggested different plant management and operational procedures. A chemometric model was developed to predict source apportionment inside the Barcelona WDS. Five different water sources were detected in water blends.
Finally, different chemometric techniques for visualization and data interpretation have been tested and evaluated for their usefulness for water quality analyses. The prediction ability of linear or nonlinear regression methods have been compared when they were used to develop empirical models and predict water quality parameters such as THMs concentrations in drinking waters, nitrates, phenols, organic matter in wastewaters, water source apportionments in water distribution system and panelists taste ratings of water samples.
Last but not least, this Thesis had as an objective to demonstrate the advantages of using chemometric methods for water quality assessment. This work showed that complex problems can be resolved using a multivariate modeling methodology with a few experiments. Therefore, this methodology is a significant improvement over unvaried approaches which are based on expensive and time-consuming measurements