Geophysical Research Abstracts
Vol. 16, EGU2014-376, 2014
EGU General Assembly 2014

Self-Organising Maps and Correlation Hunting Analysis as a Tool to Explore Patterns in Excitation-Emission Matrix Data Sets and to Resolve Dissolved Organic Matter Fluorescence Components

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Self-organising maps (SOM) have recently appeared as a powerful tool to explore patterns among the samples of large Excitation-Emission Matrix (EEM) data sets. In this paper, we propose an additional step in which the SOM analysis is conducted to perform a correlation hunting analysis on the EEM wavelength coordinates, allowing for the identification of fluorescence components. Hence, we exemplify how SOM can be used both as an analysis on the Q-mode (analysis of objects) and on the R-mode (analysis of variables). We analysed a large and heterogeneous EEM data set, including samples from a river catchment collected under a range of hydrological conditions, along a 60-km longitudinal gradient, and under the influence of a varying degree of anthropogenic impact. According to our results, in the SOM analysis on the Q-mode we could clearly discern chemical industry effluents, as well as river samples collected under flash flood conditions. On the R-mode, the correlation hunting analysis suggested the presence of four fluorescence components, occurring in EEM areas previously described in the literature. A remarkable strength that we experienced with this methodology is that outlier samples appear naturally integrated in the analysis. We conclude that SOM coupled with a correlation hunting procedure is a promising tool to study large and heterogeneous EEM data sets that, up to now, remain poorly characterised.