

Environmental Applications of Chemometrics

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ABSTRACT

By using modern instrumental methods a large number of chemical variables can be determined from a single sample. When these methods are used to monitor the environment or industrial processes large data sets are produced. E.g., in Finland the water quality of the lakes and rivers have been systematically monitored for over thirty years. Time series of the surface level fluctuation of some large Finnish lakes are over hundred years long and average precipitation data on their catchment areas have been recorded since beginning of 1900's. These kinds of data sets often contain a lot of useful information, but in order to fully exploit their potential, effective data analytical methods are needed both to extract and interpret the information. An asset of a method is if can also be used to compress and display the data in an informative way.

Principal Component Analysis (PCA), Partial Least Squares Regression (PLS) and PLS Discriminant Analysis (DPLS) have in recent years found many process and analytical applications. These methods are often useful also in studying environmental problems, especially, if the problem can be formulated as a classification, calibration or regression type problem. The application of these methods will be elucidated by several examples representing different types of environmental problems, e.g.:

- Dependence of emission of diesel engine on its running speed and load
- Effect of exposure to vanadium dust in industrial environment
- Multivariate study on urban aerosol samples
- Effects of industrial effluents in the recipient lake