

## **L02. Gray modelling approaches to investigate chemical processes**

***Roma Tauler***

*Institute of Chemistry and Environmental Research, CSIC, Barcelona, Spain*

Data modeling and data fitting in chemical sciences has been traditionally done by hard modeling techniques, i.e., data are tested against a known model based on physical and chemical laws and the parameters of this model are obtained by least squares curve fitting optimization techniques. This approach may be also called white modeling and it is valid for well known phenomena and laboratory data, where the variables of the model are under control during the experiments and only the phenomena under study affect the data. However, this ideal situation is not obeyed in many circumstances in Chemistry, especially in Analytical Chemistry, when natural samples or unknown processes are investigated. Complex phenomena like those involving macromolecular compounds or industrial processes, where physical parameters cannot be appropriately fixed are typical examples not solved by the traditional white model based data treatments. Alternative approaches have been proposed. In particular, soft or black modeling approaches attempt the description of a system without the need of an a priori model postulation, physical or/and chemical. The goal of these methods is the explanation of data variance using the minimal or softer assumptions about data. Some of these soft modeling approaches are based on Factor Analysis decompositions of experimental data. These decompositions are done by pure mathematical means and allow the identification of the number of data variance sources and often their qualitative and, eventually, quantitative estimation. Results of soft modeling data analysis are useful to validate hard modeling results and also for investigation of complex chemical systems. Pure soft-modeling (black modeling) approaches however do not provide a full characterization and knowledge of the systems and therefore a mixed soft- hard modeling approach, the so-called grey modeling approach, is desirable. In this communication, some attempts related to grey modeling using Multivariate Curve Resolution will be shown.