



Anna De Juan

Prof. Anna De Juan, Department of Analytical Chemistry, University of Barcelona, Diagonal 645, E-08028 Barcelona

Anna de Juan is an associate professor at the Department of Analytical Chemistry at the University of Barcelona since 2003, teaching chemometrics at undergraduate and graduate levels. She holds a degree and PhD in Chemistry from the University of Barcelona (UB) and her expertise is in Multivariate Curve Resolution (MCR) methods: theoretical development and application to bioanalytical and analytical problems. Since 2002 she is member of the Editorial Advisory Board of *Chemometrics and Intelligent Laboratory systems* and since 2006 of *Analytica Chimica Acta*. In 2004 she received the 4th Chemometrics Elsevier Award together with Karl Booksh. She has published more than 120 papers in international journals and books and has given more than 180 presentations in different international conferences, 50 of them plenary or keynote lectures, basically on design of chemometric tools and multivariate curve resolution developments and related methods and on applications to process analysis, hyperspectral image analysis and general analytical applications.

The many faces of Chemometrics in the PAT world !

The role of Chemometrics in the recent decades has been essential to improve the performance and control of industrial processes and the quality assessment of final products. Process understanding has used classical hard-modeling and soft-modeling approaches, but the development of hybrid approaches that simultaneously include first principles knowledge and allow for deviations from the ideal model behavior has become particularly suitable in the industrial context. Data fusion is another pillar in process modeling and control. Indeed, process control involves most often outputs of several sensors different in nature and amount of information and strategies to get efficient data fused structures for process control are of utmost importance.



Data fusion has to be interpreted in a wide sense, not only referring to merging the output of several hard sensors, but to use diverse outputs from soft sensors that may come from the same instrumental measurement. On-line control of process evolution no longer needs to be attached to rigid approaches requiring batch synchronization. The natural batch-to-batch variability can be respected and flexible Multivariate Statistical Process Control (MSPC) approaches based on local models are proposed for this purpose. Finally, product quality assessment was classically identified with the quantitative analysis of certain physicochemical properties. Nowadays, more global quality attributes, such as product heterogeneity, are of interest, and require new analytical and data analysis approaches. In this respect, the use of advanced analytical techniques, such as hyperspectral imaging, combined with concepts coming from other fields of knowledge, such as the Theory of Sampling (TOS), are good ways to provide the sought information. Most aspects mentioned above will be tackled through real industrial examples that illustrate the potential of the approaches described.