

9th Chemometrics Symposium of the Belgian Chemometrics Society

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On April 11th 2008, the 9th Chemometrics Symposium of the Belgian Chemometrics Society was held at the Centre Wallon de Recherches Agronomiques (CRA-W) in Gembloux (Belgium), a TRACE WP2 partner. The morning session, chaired by **Bieke Dejaegher**, started with a short introduction of the CRA-W by **Vincent Baeten**.

Then **Bas van den Bogaert** (CQ Consultancy, Leuven, Belgium) gave a lecture, entitled “A chemometrical perspective on the analysis of micro-array data”. Bas van den Bogaert obtained a PhD in Chemometrics at the University of Amsterdam, worked for some time as a chemometrician at Solvay in Brussels, and since 2002 at CQ Consultancy in Leuven. His major fields of expertise are experimental designs and signal processing. In his talk, he discussed the application of several chemometric techniques, i.e. Partial Least Squares (PLS),

Support Vector Machines (SVM), Radial Basic Function PLS (RBF-PLS), Continuum Regression (CR), Gradient Directed Regularization (GDR) and Random Forests (RF), in the analysis of micro-array data. For small data sets, he recommended a double-loop cross validation to avoid overfitting and over-optimistic results.

Peter Goos (*Universiteit Antwerpen, Belgium*) discussed “Optimal design for split-plot experiments”. In 2001, Peter Goos obtained a PhD in the field of econometrics and statistics at the Faculty of Applied Economic Sciences of the University of Leuven. Since 2004, he is Professor at the Faculty of Applied Economic Sciences of the University of Antwerp. His major fields of expertise are optimal experimental designs and General Linear Models. In his presentation, he explained the usefulness of split-plot or even split-split-plot type of experimental designs, in situations where many experiments span several steps of a production process and/or involve factors whose levels are hard to change. He showed how such experiments can be designed, and also their advantages and disadvantages for industrial applications were discussed and illustrated.

The last speaker of the morning session was **Sébastien Gourvéné** (*GSK, PAT&C, GlaxoSmithKline R&D, UK*), who presented “Industrial PAT applications of multivariate analysis”. In 2005, Sébastien Gourvenec obtained his PhD in Pharmaceutical Sciences at the department of Professor Massart with a thesis on “Chemometric methods for batch process control”. He is currently working at GlaxoSmithKline Research & Development in Stevenage (United Kingdom), at the Process Analytical Technologies (PAT) and Chemometrics section. He presented an overview of the motivation for PAT techniques in the pharmaceutical industry and the use of some chemometric techniques for developing, monitoring and controlling robust processes. Examples of PAT applications of different unit operations (chemical reaction, distillation, drying) were given.

The three presentations of the morning sessions were followed by one-minute poster introductions.

In the afternoon session, chaired by Bas van den Bogaert, **Lutgarde Buydens** (*TRACE WP6 partner, Radboud University Nijmegen, IMM Analytical Chemistry, The Netherlands*) talked about “Chemometrics for food authentication”. After studying pharmacy and informatics, Lutgarde Buydens obtained her PhD in Pharmaceutical Sciences at the department of Professor Massart in 1986. Since 1989, she is Professor at the Radboud University Nijmegen. She received the first Elsevier Chemometrics Award in 1992 for noteworthy accomplishments in the field of chemometrics by younger scientists. During her presentation, she discussed the importance of tracing the authenticity of food, both for the consumers and

the producers, leading to the introduction of food-quality certifications based on geographical origin by the European Commission, such as, for example, the Protected Designation of Origin (PDO). Since labeling claims are rarely supported by analytical data and since compliance monitoring is based solely on paper auditing procedures, she emphasized the importance of the TRACE project, that intends to develop analytical methods that provide fingerprints of food products, integrated in generic traceability methods and systems, that will provide consumers with added confidence in the authenticity of European food products. The lecture explained the position and role of chemometrics and statistical methods in the project and some case studies were presented.

Then, the 2nd D.L. Massart Award in Chemometrics was granted to **José Camacho** (*Technical University of Valencia, Dept. of Systems Engineering and Control, Spain*), for his thesis entitled “New Methods Based on the Projection to Latent Structures for Monitoring, Prediction and Optimization of Batch Processes”. Promotors of the thesis are Profs. J. Picó and A. Ferrer.

He discussed the application of methods based on the projection to latent structures, such as Principal Component Analysis (PCA) and PLS, to batch processes, and moreover the modeling of batch process data using bilinear PLS-based methods. The multi-phase modeling structure was proposed, which can be adjusted according to the process dynamics, leading to a better process understanding and performance improvement in applications, such as monitoring and prediction. He presented a new set of tools to calibrate, analyze and handle multi-phase models, i.e. the Multi-phase Framework, which includes a new pattern recognition algorithm, the Multi-phase algorithm, new PCA and PLS cross-validation methods, designed after extensive investigation of the cross-validation technique, and Analysis of Variance (ANOVA). During the talk, several applications were presented.