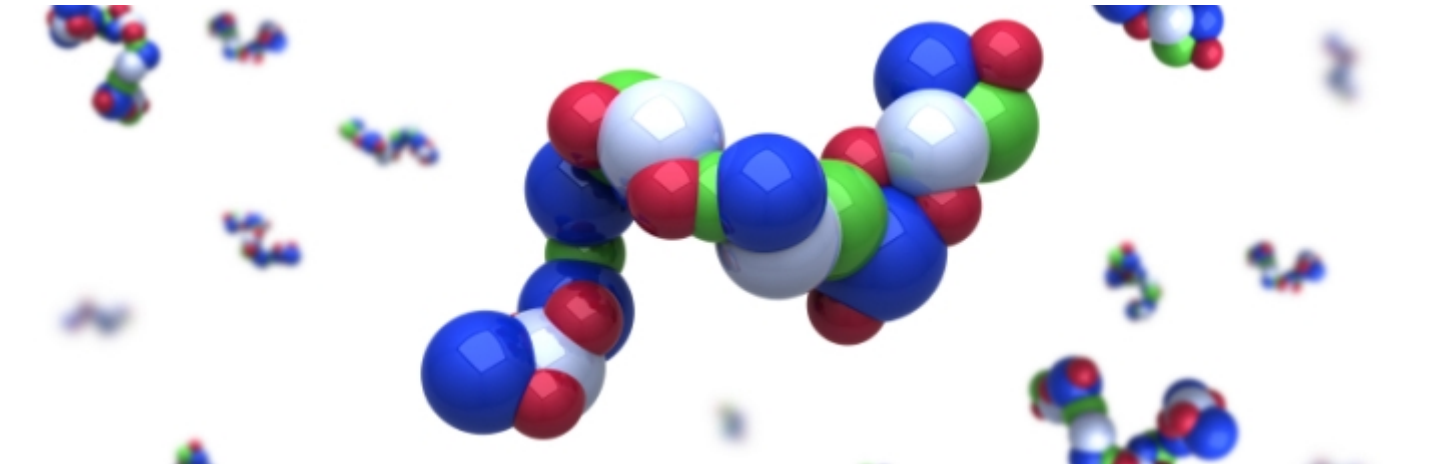

Improving prediction robustness from hard and soft modeling

Jplus Consulting was formed in 2009 to develop and commercialise innovative multivariate data analysis tools for the quantitative characterization of chemical processes. The ReactLab™ suite of software provides sophisticated but easy to use applications for analysing both process and equilibrium titration spectroscopic measurements and yields all the underlying reaction rates, equilibrium constants as well as the spectra and concentration distributions of the participating chemical species.

Working with an industry leader

Dr Peter King, Managing Director of Jplus Consulting, says "Very early on we started a dialog with CAMO Software who recognized the complementary nature of our 'hard modeling' approaches to the classical chemometric multivariate analyses such as PCA and PLS and 'soft modeling' techniques included in The Unscrambler® X."

Essentially both approaches analyse chemical data to gain information about the underlying process or system using mathematical and statistical tools. The key difference is that the chemometric algorithms do not require a starting model but allow the development of an abstract model from patterns and behavior in training samples which can then be used to predict the constitution and key characteristics of unknown samples. These characteristics may not be 'real' parameters such as absorption spectra or concentration profiles but abstract mathematical decompositions, which nonetheless allow very powerful prediction of unknowns. "The Unscrambler® X is very well equipped in this area and offers a wide range of tools in an exceptionally user friendly environment" says Peter.

Rigorous mathematical model for chemical processes

'Hard modeling' starts with a mathematically rigorous model of the process under investigation. In the case of ReactLab, this is the reaction scheme underlying a chemical process. This model is then fitted to the measurement. This involves the adjustment and optimisation of the key rate and equilibrium parameters using a least squares approach. This yields the fundamental reaction parameters that define the process which can be re-used in more complex systems and by other researchers.

ReactLab™ is an ideal tool for studying dynamic chemical systems, either kinetics, where reactions are monitored spectroscopically as a function of time in order to determine rates and yields of a process, or chemical equilibria, where the data are collected during titration experiments in order to quantify ligand binding interactions or complexation equilibria. "We're looking at specific cases with CAMO where the marriage of these two approaches can be brought bear on process monitoring applications involving robust characterization of the process in the lab, coupled with online spectroscopic measurement of the subsequent process. By applying a combination of ReactLab™ & The Unscrambler® X methods we aim to provide robust online predictions of component distributions and process quality" explains Peter.

Industry:

- Multivariate data analysis software vendor

Product:

- The Unscrambler® X and ReactLab™

Executive Summary:

- Specialise in 'hard modeling' approaches to multivariate data analysis for the study of dynamic chemical systems
- Data may comprise spectroscopic measurements derived from kinetic studies or collected during equilibrium titration experiments
- Working with CAMO to offer software tools to complement the classical techniques used in chemometric multivariate analyses such as PCA and PLS
- Chose to partner with CAMO Software due to the powerful tools and user-friendliness of The Unscrambler X and their focus on innovation in multivariate analysis field

At a glance: Jplus Consulting

- Founded in 2009 by Dr Peter King and Associate Professor Marcel Maeder, co-author of the textbook 'Practical Data Analysis in Chemistry' Elsevier 2007
- Based in Perth, Western Australia and servicing clients worldwide
- Core product family, ReactLab™ used for the analysis of multivariate spectrophotometric chemical process data in order to quantitatively characterize underlying fundamental reaction mechanisms
- Applications in both academic and commercial research and development as well as process monitoring and quality control

"By applying a combination of ReactLab and The Unscrambler methods we aim to provide robust online predictions of component distributions and process quality"

Dr Peter King
Managing Director, Jplus Consulting

A winning combination

Combining ReactLab™ analysis with the variety of methods available in The Unscrambler® X allows a user to extend beyond the boundaries offered by either approach alone. Peter believes this dual approach can benefit both company's clients. "There are times when the measurement does not lend itself to complete interpretation by one analysis or the other but together ReactLab™ and The Unscrambler® X extend the reach and flexibility of your options. In our view this is very much a case of 'the whole being greater than the sum of its parts'" he explains.

"We are delighted to be working with CAMO Software" adds Peter. "Their clear insight into developing strategic partnerships with other MVA innovators is, in our view, the only way to stay at the forefront of these multivariate analytical technologies. The need for a wide repertoire of techniques to get the most from the vast amounts of data that are generated by modern instrumentation and process monitoring technologies can only drive exciting and innovative progress in this area."

By combining the complementary strengths of two leading multivariate analysis solutions, Jplus Consulting and CAMO Software are working together to deliver even greater value to their clients.

Jplus consulting
multivariate analytical technologies

For more information on Jplus consulting please visit
www.jplusconsulting.com

CAMO

For more information on our full range of solutions please visit
www.camo.com

Try The Unscrambler® X in your web-browser

Free TestDrive