PAC

Process Analytical Chemistry - Data Acquisition and Data Processing

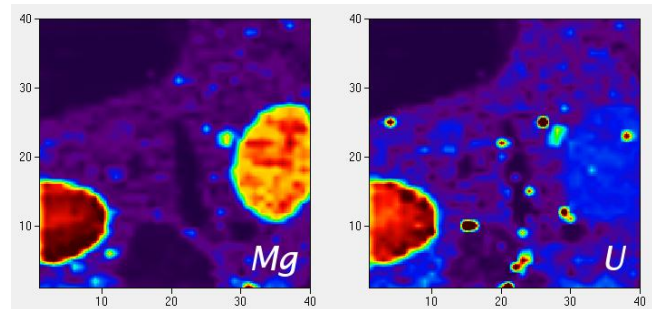|	
Main location	Linz (Upper Austria)
Other locations	Kundl (Tirol), Salzburg, Lenzing (Upper Austria), Krems (Lower Austria), Vienna
Thematic field	Gaining valid chemical information directly from the process streams of chemical and biochemical industry, inline and in real-time.

Success story summary

SW-Tool IMAGELAB: analyzing images with a chemist's eye

Within the K-project PAC a software tool for the researchers was developed in cooperation with external partners. Although this tool is not yet ready for the market there has already been great response of the users. Through practical usage the future SW-product can be optimized by the inputs and requirements of the researchers. There is also an advantage for the project itself, as the tool can be specified according to the needs of the network partners.

Success story

A main research field of the K-project PAC is the chemometric analysis of spectral data. This means that the raw data produced by a spectrometer have to be prepared and analyzed with mathematical and statistical methods in order to extract the desired chemical information. Researchers in the PAC-network are developing novel methods of "chemometric modeling" to perform these tasks.

PAC also focuses on processing and interpretation of multidimensional spectral images (also called Hyperspectral Imaging). This means that a photo of an object is taken which does not only register single color dots but one or more spectra at each pixel of the photo. The contained information is converted into pictures by means of multivariate methods, reflecting the desired chemical information. Such "hyperspectral photography" produces large amounts of data which only can be processed with appropriate software support.

Cross section through concrete, ICP/MS coupled with ImageLab. Left magnesium, right uranium. You can see that the left dolomite grain is interspersed with uranium. Data: M. Bonta/A. Limbeck, TU Vienna

The available tools have a big impact on the efficiency and quality of the results. In an optimal constellation for both partners a commercial software development effort could be tightly connected to the K-project. The researchers in PAC have full access to a tailor made computer program at a very early stage. The program exactly covers the researchers' practical needs as their requirements were integrated into the software-design from the very beginning. Moreover, a tool that already triggers enthusiasm among the specific group of testers and "beta users", is almost certainly going to be commercially successful in the nearest future.

Impact and effects

Due to a new SW-Tool, which was developed in the K-project in collaboration with external partners, highly efficient and qualitative research in the field of data processing of hyperspectral imaging data processing is possible. By the use of this tool technologies for generating spectral images can be developed and optimized effectively.

Contact:	K-Project PAC – Process Analytical Chemistry
	RECENDT GmbH, Robert Holzer
	Altenberger Straße 69, A – 4040 Linz
	+43 (732) 2468 - 4602
	robert.holzer@recendt.at www.recendt.at