

## **L02. Advanced process modeling with Multivariate Curve Resolution**

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Multivariate curve resolution is a powerful tool to model complex processes. The underlying bilinear model of curve resolution, which expresses the raw data collected during process monitoring as the composition-weighted sum of pure component signal contributions, adapts to the description of processes collected with a variety of spectroscopic techniques and with partially or completely unknown mechanisms.

Curve resolution can easily handle multitechnique and/or multiexperiment data structures. The analysis of these data sets provides a very robust structural information to characterize the compounds involved in a process (multitechnique monitoring) or can allow for the simultaneous study of a set of designed experiments that can allow for the detection of minor or intermediate compounds or for the assessment of the effect of different inducing agents or process control variables in the process mechanism. Multiset arrangements are also the key strategy to tackle problems of rank-deficiency, i.e., resolution of compounds with identical spectral shapes in a particular technique or identical concentration profile shapes in certain experimental conditions.

Introducing external information related to properties of the signal recorded or to the shape of the process profiles, when available, is a capability of CR methods. Whereas soft-modeling constraints (non-negativity, closure, ...) are applied since long in process modeling, process profiles can also be fitted according to a hard model, if the mechanism of the process is partially or totally known. Unlike pure hard-modeling approaches, where the total mechanism of the process should be known and a global model is needed in multiexperiment analysis, hard-modeling constraints can fit only some of the compounds contributing to the signal recorded during a process and can handle sets of experiments with a non-common model or structures with model-free and model-based experiments. All these possibilities will be shown with real examples.