SL09   Chemometrics for Process Modeling and Control of Pharmaceutical Products

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Nowadays, production and control of pharmaceutical products must fulfill many regulatory issues. This is the reason why every time becomes more important to provide reliable data analysis tools that may handle all kinds of measurements produced during process monitoring and control.

Multivariate resolution is a chemometric tool that allows describing the raw spectroscopic measurements linked to a process or to the characterization of a product into the basic contributions of the compounds involved. This methodology, notably the algorithm Multivariate Curve Resolution-Alternating Least Squares (MCR-ALS) [1], allows treating information from different experiments and techniques simultaneously and allows accommodating information as diverse as physicochemical or calibration models.

The application of this tool will be demonstrated in the process modelling area, where examples of drug degradation or transformation monitored in solution by spectroscopy and chromatography [2] or in solid form by hyperspectral imaging [3] will be shown.

Within the area of process control, MCR including an internal calibration model will be applied for the determination of the end-point of a blending process monitored by NIR [4]. Finally, the characterization of solid end products by combining hyperspectral images and MCR will show the potential of this methodology for quantitative analysis and description of formulation heterogeneity [5].

References

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