LECTURE

Multivariate resolution for NIR image and process analysis

Anna de Juan

Anna.dejuan@ub.edu

University of Barcelona, Barcelona, Spain

Sara Piqueras[1], Sílvia Mas[1], Joaquim Jaumot[2], Jean Michel Roger[3], Benoît Igne[4], Romà Tauler[2].

1. Universitat de Barcelona.
2. IDAEA-CSIC. Barcelona.
3. CEMAGREF. Montpellier.
4. GlaxoSmithKline, Pennsylvania, US.

Multivariate resolution designs a family of chemometric methods used to interpret the information contained in multicomponent systems. NIR spectra do not often provide selective information about compounds and, therefore, tools to unmix the information related to a particular measured signal are particularly suitable for this kind of spectroscopic measurement.

Different examples dealing with NIR-monitored images and processes will be presented and multivariate resolution with the adequate preprocessing and postprocessing will show the variety of information that can be gathered from the application of this kind of methodology.

Image analysis of pharmaceutical mixtures is a classical problem. Multivariate resolution in multiset analysis mode will allow treating simultaneously several images with complementary compositions. The resolved pure spectra and distribution maps will allow for the identification of compounds, the quantitative global and pixel-wise analysis of mixtures and the global or compound-wise assessment of formulation heterogeneity[1].

Process analysis is also a common area for NIR monitoring. Two examples will illustrate this fact. On the first one, a blending process will be modelled by multivariate resolution applying a correlation constraint, which allows for using internal calibration models in the process modeling. Blending trajectories for each of the compounds in the system will be obtained and, therefore, a more detailed global or compound-wise assessment of the blending end-point will be obtained. Besides, an integral vision of the global blending evolution is attained[2].

The second process example will use variations of the intense NIR water band to monitor indirectly a colloidal process. Indeed, water forms can change when they solvate a more or less disperse colloidal phase. The kinetics of a gel formation process will be interpreted by using NIR difference spectra and multivariate resolution in the variant of the hard- soft-modeling algorithm. Working in this way, a kinetic model can be proposed that explains the gel formation behavior and an additional soft-modeling contribution can account for the variations of the signal due to scattering changes in the heterogeneous medium[3].

REFERENCES

1. S. Piqueras, J. Burger, R. Tauler, A. de Juan. Relevant aspects of quantification and sample heterogeneity in hyperspectral image resolution. Chemometrics and Intelligent Laboratory Systems, 117 (2012) 169-182.
2. J. Jaumot, B. Igne, C.A. Andersson, J.K. Drennen, A. de Juan. Blending process modelling and control by Multivariate Curve Resolution. Talanta, 117 (2013) 492-504.
3. S. Mas, R. Bendoula, G. Agoda-Tandjawa, A. de Juan, J.M. Roger. Study of time-dependent structural changes of laponite colloidal system by means of near-infrared spectroscopy and hybrid hard- and soft-modelling multivariate curve resolution alternating least squares. Chemometrics and Intelligent Laboratory Systems, 142 (2015) 25-292.