Orthogonalisation method for robustness improvement of online NIR applications

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On-line model maintenance is one of the main problems when developing Near Infrared Spectroscopy (NIRS) applications. Perturbation appearance due to environmental changes, maintenance operation or aging of the instrument often affects the model performances. Model corrections with classical methods such as bias and slope or model redevelopment are not always satisfactory. The use of an orthogonalisation method can be a very effective way to solve this problem; this approach is illustrated in this study with an industrial application.

The monitoring of a polyamide polymerization by NIRS is a well-known subject which gives excellent results. A PLS model can predict directly the end of the polymer chain concentration, or less directly the product viscosity. It provides the real-time monitoring of the polymerization process. However, after several years of operation, an unidentified perturbation appeared, leading to the failure of the model during several months. The purpose of Dynamic Orthogonal Projection (DOP) is to make the model independent from perturbations, without any standardization set available. Indeed, when performing on-line process measurements, it is impossible to gather the measurements of the same samples measured before and after perturbation in such a standardization set. Thus, the principle of DOP is to reconstruct spectra as if they had been measured before perturbation. Only a small number of samples is needed to model the perturbation space.

DOP has been applied with success to correct the model with only a few samples, whereas model redevelopment was not entirely satisfactory. Furthermore, the study of DOP spectroscopic corrections was analyzed and feedback to the process to improve it.

Maintenance and robustness issues of predictive models in NIRS are a real restraint for its expansion into the industrial world. DOP is a mathematical solution which overcomes the impact of perturbations with only a few samples.