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Improve inline NIR model robustness with Dynamic Orthogonal Projection method

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1 Introduction

Online 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.

2 Material and methods

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 failureof the model during several months.

This application is an ideal case for applying Dynamic Orthogonal Projection (DOP) [1]. The purpose of this chemometric method is to make the model independent from perturbations, without any standardization set available. Indeed, when performing online process measurements, it is impossible to gather the measurements of the same samples measured before and after perturbation in such a standardization set.

3 Results and discussion

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. This is done by a PCA, based on spectral differences between real and reconstructed spectra. The calibration database is then projected orthogonally from this space and the model is rebuilt. The corrected model is still robust when the perturbation appears or disappears.

4 Conclusion

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 an elegant mathematical solution which overcomes the impact of perturbations with only a few samples.

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