Discrimination strategies for polymer identification for continuous processes with on-line Near Infrared Spectroscopy

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Methods such as near infrared (NIR), provide fast and precise results. During continuous process control, in the frame of PAT (Process Analytical Technology) in the chemical industry, NIR analysis is able to monitor transitions from one product to another, and to isolate compliant products from those affected by the transition. In these cases, exhaustive models for quantitative prediction are not precise enough. It is then important to determine first the product, in order to choose its specific quantitative model, and then to predict the end of the transition toward a stable state.

The study has been conducted on polymerization processes with a transition from one polymer to another. NIR spectra (12 000 - 4 000 cm^{-1}) have been acquired on-line during the whole process. The stable state spectra have been used for building models, and an independent spectral set, corresponding to the entire transition, has been used to test them. Several discrimination approaches have been compared: PLS-DA (Partial-Least-Square Discriminant Analysis) with 3 different strategies: direct approach, hierarchical, or “one versus all”; and SIMCA (Soft Independent Modelling of Class Analogy).

This study has developed a discrimination strategy for polymer identification during the transition phases, with on-line NIR in the chemical industry. The importance of the chemometric method choice has been illustrated. It strongly depends on data, discrimination difficulty, application, and objectives pursued.