Discrimination Strategies For Polymer Identification For Continuous Processes with On-Line Near Infrared Spectroscopy

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1 Introduction

Methods based on vibrational spectroscopy, and specifically near infrared (NIR), provide fast and precise results. During continuous process control, NIR analysis is able to monitor transitions from one product to another, 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 to choose its specific quantitative model and then to predict the end of the transition toward a stable state.

2 Material and methods

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) [1] with 3 different strategies: direct approach, hierarchical, or “one versus all”; and SIMCA (Soft Independent Modelling of Class Analogy) [2].

3 Results and discussion

The study showed that hierarchical discriminant analysis allowed to better differentiate similar classes. However, this approach isn’t adapted to transitions, because spectra in transition contain chemical information that is not necessarily taken into account in the sub model. “1versus all” models are less accurate but they provide the adequate observation of transition kinetics. (C.f. figure 1). In both of these approaches the models can be optimized independently, which is not the case for direct approaches. These methods have also been compared to SIMCA modeling.

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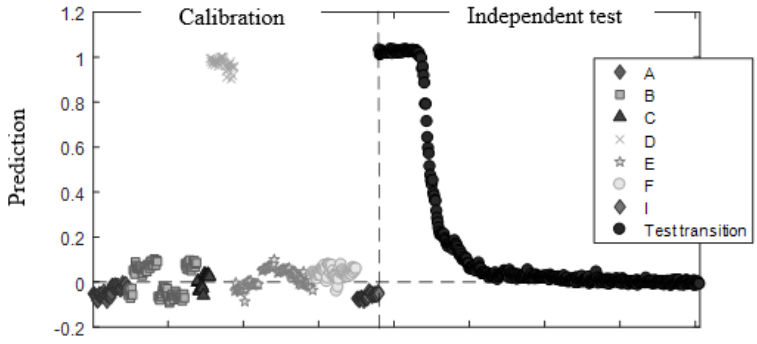

Figure 1 – Example of model "Class D versus all" with prediction in calibration (left) and for an independent test set (right), showing the transition kinetic.

4 Conclusion

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.

5 References

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