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Orthogonalisation Method For Robustness Improvement of In-line NIR Applications

CONTEXT

Issues: Model robustness and maintenance when applying Near-Infrared Spectroscopy (NIRS) for online monitoring

How to build a robust model ? ➔ orthogonalisation methods

Industrial application: Monitoring of polyamide viscosity by NIRS

- ☺ **PLS prediction for process real-time monitoring used in routine**
- ☹ **After several years of operation, an unidentified perturbation appeared, leading to PLS model failure**

Objectives :
- ✓ **Process Monitoring : build a robust model to cope with such variations**
- ✓ **Process Understanding : find out what went wrong in the process**

Measurement in diffuse reflectance of powders

MATERIAL & METHODS

Process: Solid phase polymerization of powders

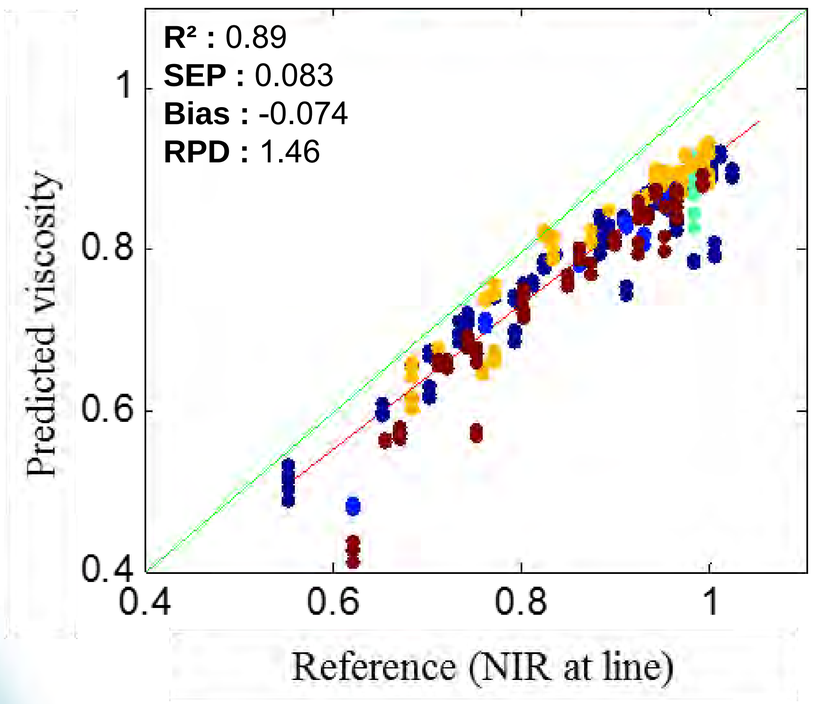
- Reference method ➔ Viscosity measurements in solution (1 to 2h duration)
- Secondary method ➔ NIRS

Methods: Application of Dynamic Orthogonal Projection (DOP)

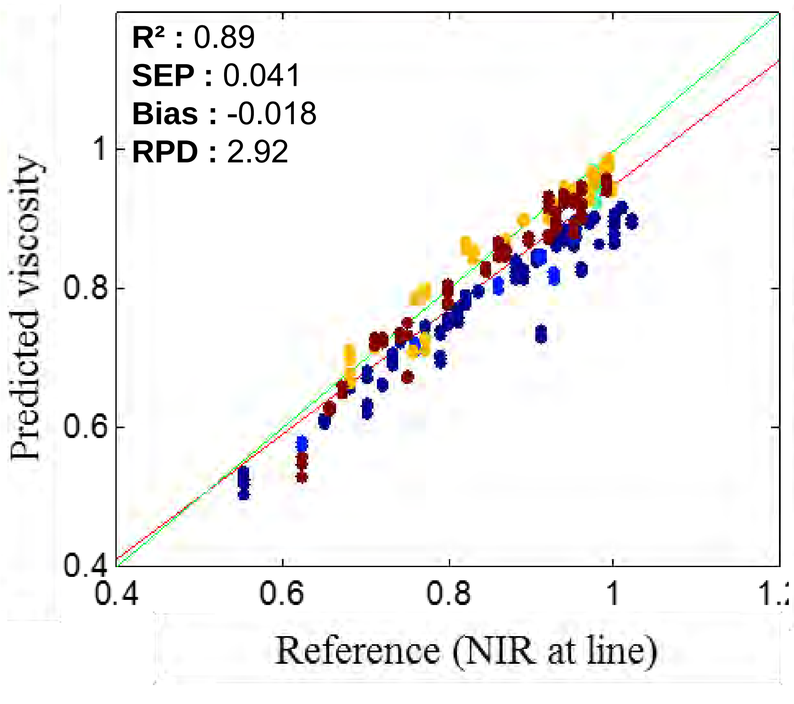
- **Calibration set :** 2008-2013
  - **1. Original model :** 2008-2013
  - **2. Exhaustive model** : all samples from 2008-2014
  - **3. DOP model :** only 20 samples from 2014 used for orthogonalization
- **Independent Test set** : 2015

RESULTS on TEST SET & CONCLUSIONS

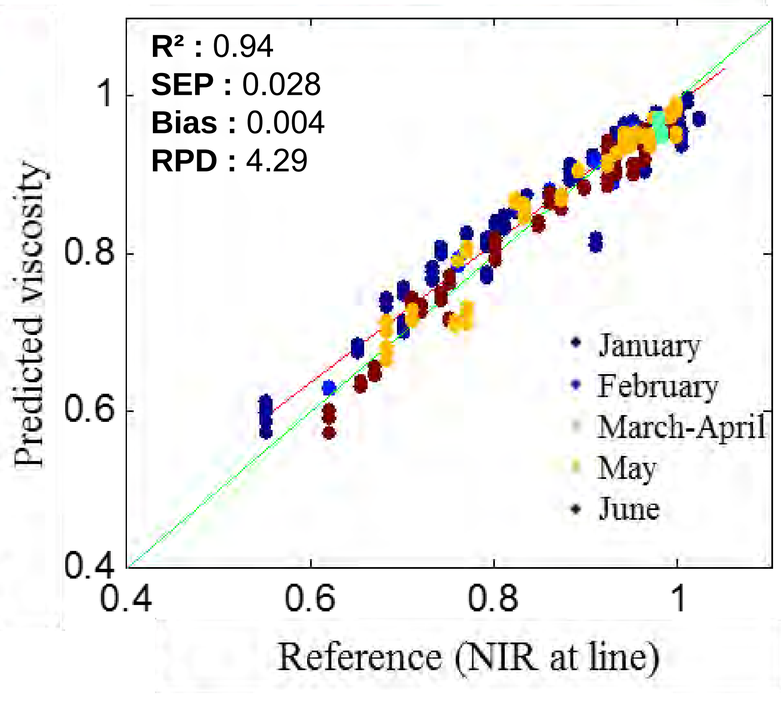
1. Original model



2. Exhaustive model



3. DOP model



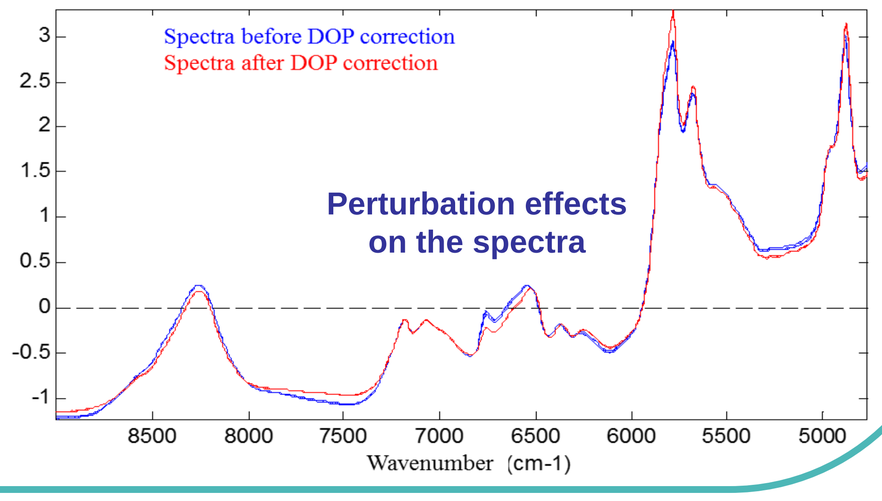
☺ **DOP uses fewer samples than exhaustive model required**

☺ **In this study, DOP outperforms the exhaustive model**

☺ **DOP allows a diagnostic of the perturbation**

☹ **Not available in commercial software**

☹ **Requires chemometrics expertise**



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