



Spectroscopic (NIR) Calibration

WHY SPECTROSCOPIC CALIBRATION?

The last few years more and more companies opt for (on-line) NIR calibration models as an alternative to time-consuming and expensive lab analyses. This is often the case throughout the whole production process: to check the quality of the feedstock at delivery, to obtain timely information on different process streams, and to quantify the quality of the end product.

Due to continuous chemometrical developments, the number of applications of spectroscopic calibration - especially NIR - continues to increase, despite the strong overlap of spectral bands and peaks in the NIR region.

COURSE SET-UP

In this course we will go through the different steps required for a successful Spectroscopic Calibration: from sample selection over validation and interpretation of the models, up to guidelines and recommendations for the maintenance and update of calibration models in the future. Since emphasis will be put on practice, theoretical aspects will be alternated with practical exercises.

COURSE OBJECTIVE

In this course, the participants will develop a feel for the multivariate approach to spectroscopic calibration, gain insight into the underlying methods, learn to perform a multivariate calibration in "normal" situations and recognise problem situations.

INTENDED AUDIENCE AND PRIOR KNOWLEDGE

If your aim is to perform multivariate calibrations and/or to properly interpret the results, this course will satisfy your needs.

No prior knowledge is required.

PRACTICAL

Each course day will be held from 9 am to about 5 pm. The course dates and fees are listed on the attached application form. The course fee includes handouts and lunches.

To apply, send us back the application form, or apply on-line, at least 20 days before the start of the course .



COURSE CONTENTS

Day 1:

- NIR introduction
- Exploratory Multivariate Analysis
 - Visualisation of information in big data sets
 - Principal Component Analysis (PCA)
 - Cluster analysis: searching for groups of similar samples

Day 2:

- Basic principles of calibration techniques
 - Multiple Linear Regression (MLR)
 - Principal Component Regression (PCR)
 - Partial Least Squares (PLS)
- Interpretation of calibration models
- Model validation
- Preprocessing and scaling of spectra

Day 3:

- Detection of outliers and non-linearities
- Prediction with calibration models
- Selection of calibration samples
- Standardisation of calibration models
- Monitoring the performance of (on-line) calibration models