Feed analysis using NIR spectroscopy

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Rapid and accurate laboratory analyses of rape seed, silage maize and compound feeds has long been recognised in our laboratory. Near Infrared Reflectance (NIR) Spectroscopy offers very good solution which can replace the conventional labourious and time-consuming methods. Near infrared analysis is based on the development of calibration equations that reflects the relationship between the constituents of the sample and NIR spectral information. The objective of this paper was to present our results from the development of the calibration equations in the field of variety testing and compound feed analyses.

Calibration databases should include enough samples to cover most of the possible spectral variability encountered during routine analysis and to predict the constituents of unknown samples accurately. Our laboratory collected sufficient number of samples for calibration from graphically different sites of the whole Czech Republic and also with different genetic backgrounds. This fact resulted in a robust calibration.

Another assumption of a good calibration is a suitable software. The basic software of NIRSystem 6500 was extented by Software NIR calibration 1.0 (EFFICHEM, CZ) which allows to develop calibration equations with better qualitative parameters.

Calibration equations quantify the relationships between NIRS and laboratory reference methods. The accuracy of the conversion can be expressed as a standard error of the prediction. Prediction of unknown values from NIR spectra is not a simple task.

The spectra produced by the NIR instrument represent the total chemical and physical properties of a sample. Chemical information appears at specific locations in a spectrum. Physical properties of a sample, as a particle size, are eliminated by mathematical corrections as standard normal variate (SNV) or multiplicative scatter corrections(MSC). Principal component analysis (PCA) reduces the spectral information into a smaller number of independent factors. After this simplification the model can be used for the development of calibration equations by principal component regression (PCR). Partial least squares (PLS) regression is similar to PCR, but uses the chemical information to form factors for calibration equations which are able to describe the chemical information.

In PCR the factors are formed without the chemical information and explain the spectral variation. Both PCR and PLS require cross-validation to prevent overfitting. Cross validation obtains validation errors by partitioning the calibration set into several groups.

Calibration should always be evaluated with an external test set : outlier detection, nonlinearity detection, Hopkins statistic to evaluate the clustering tendency, etc.

650 compound feed samples from 7 regional laboratories of our institute collected during the last two years were used for the study. All the samples were ground (1 mm). Measurements were carried out using a FOSS NIRSystem 6500, a near infrared reflectance spectrophotometer in the 1100 – 2500 wavelenghts range. Samples were measured in small ring cups cuvets. The results are summarised in the *Table 1*.

Conclusions

NIRS proved to be a suitable technique for checking and testing laboratories. NIRS enables determination of wide range of analytical parameters in very short time with an acceptable precision and accuracy especially when a new powerful data processing is applied.

References

JOHN S.SHENK, MARK O.WESTERHAUS – Analysis of agriculture and food products by Near Infrared Reflectance spectroscopy

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Table 1: **The relationships between NIRS and the classical methods for compound feeds**

Parameter	Range (g/kg)	Error of prediction (classical method)	Error of prediction (NIR method)	**Correlation coeficient**
PROTEIN	to 160	4 g/kg	5 g/kg	0.91
	from 160 to 320	2.5 % rel.	3.1 %	0.94
FAT	from 4 to 100	4 g/kg	3.2 g/kg	0.97
Crude Fiber	from 4 to 100	4 g/kg	6.0 g/kg	0.92
STARCH	over 200	10 g/kg	14.3 g/kg	0.81

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