Implementation of on-farm NIR

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The Regional Service for Agro-food Research and Development (SERIDA) is a research public body of the Principality of Asturias (Spain), created which aims to contribute to the modernization and improvement of the capacities of the regional agro-food sector.

In the north of Spain dairy farms have undergone an important restructuring process in the past decades. Active farms need to minimize cost and increase efficiency and the use of fresh and preserved forages with high quality play an import role as nutrient supply. The characterization of forages is the key factor in the formulation of diets and animal performance, because poor quality forage can further reduce intake and give only a small net gain or milk production.

In the Nutrition Laboratory of SERIDA, NIR spectroscopy has been used successfully for many years to determinate major chemical and fermentative parameters on dried and wet forages by using laboratory pre-dispersive instruments. The chemical and NIR analysis are performed under the requirements of ISO/IEC 17025.

Recent progress in NIR instrumentation enables the use of this technology at industrial level and outside the laboratory. These instruments are useful for process measurement because they are more rugged and better suited to in-line or on-site applications, even under aggressive conditions. However, to develop new calibration models is not a simple task; it needs a large data base. Spectrophotometers, even of the same type, can vary both in wavelength calibration and photometric response. This is due to tolerances, differences in optics, detectors and light sources, changes over time in the instrumental response, etc. When the instruments are different, much greater variations can be expected. These differences mean that calibration equations developed on one instrument will not usually perform satisfactorily on another unless they have been deliberately designed or corrected to do so.

In recent years the studies conducted in our research group have been focused on examining the possibility of successfully transferring undried forage calibrations from a dispersive at-line NIR instrument to a diode array on-site NIR instrument or handheld instrument. This was done using a transfer method as simple as possible, to establish controls at farm level, to improve food security, economic viability, and social sustainability of grazing lands and the livestock industry for rural communities.

Standardization of two NIR instruments, one pre-dispersive and another one an on-site post-dispersive diode array, to transfer from one to other calibration models to predict fermentation parameters of wet silages.

Example 1

Instrument 1: NIRSystem scanning monochromator provided with a transport module in the scanning range of 400 to 2500 nm at 2 nm interval. The spectral data were recorded in reflectance mode (log 1/R) using calibration software. The analyses were carried out using natural cells; two different charges of each sample were scanned in duplicate, averaging the resulting spectra.

Instrument 2: On-site diode array spectrometer with a scanning range from 400 to 1680 nm with data recorded every 3 nm in reflectance mode (log 1/R).The analysis was carried out using a Petri dish to contain the wet samples. With an integration time of 100 ms, 20 scans were averaged for each measurement. All spectra were recorded using calibration software.

This study has been developed with three hundred and forty four (N=344) grass silage

samples, collected from different farms, across North Spain. As a first step we developed the calibration models on instrument 1, after trim, to predict dry matter content and fermentative parameters: pH, ammonia-N and lactic acid and volatile fatty acids. After that, the calibration developed provided good results for external validation spectra scanned in instrument 2, applying a standardization matrix, using five wet silage samples and giving GH and NH average values (0.80 and 0.24, respectively) and SEP< 1.3*SEC, became acceptable within the control limits.

This study demonstrates that calibration models already available for laboratory instrument on wet silages, the most difficult sample type due to sample presentation (wet and large fibers), to predict fermentative parameters, present in low amounts, can be transferred to on-site diode array instruments allocated in different countries or farm points as real time sensors for fermentative process control.

Example 2

A somewhat different approach involves orthogonalizing the spectra in the calibration set to sources of variability in the transfer set, and then redeveloping the calibration. In transfer by orthogonal projection (TOP) (Andrew & Feran, 2004) the calibration spectra are orthogonalized to principal components derived from the set of different spectra for the transfer set. This will produce a calibration that accommodates the differences between the instruments as observed in the transfer set, though there may be some loss of performance if the orthogonalization also removes some of the signal useful for prediction.

In this case as a first step towards implementing quality control on farm and country level using diode array on-site NIR instruments, the present work has examined the possibility of successfully transferring undried silage calibrations from a dispersive at-line NIR instrument (Instrument 1) to a diode array on-site NIR instrument (Instrument 2) to predict dry matter content, crude protein by Kjeldahl analysis, and neutral detergent using 564 wet silage forage samples.

Two approaches for calibration transfer were used. The first was simply to standardize the spectra of Instrument 2, by subtracting the mean difference spectrum calculated from the 10 samples. The second was to remake the calibration of Instrument 1 after orthogonalizing all the spectra in the calibration set to principal components derived from the 10 different spectra to use TOP, as well as applying the mean difference correction to the spectra from Instrument 2.

This study has established that it is possible to successfully transfer calibrations, using TOP, to predict nutritive parameters on intact grass silages from an at-line instrument (Instrument 1) to an on-site NIR instrument (Instrument 2). In particular, neither cutting the spectral range of the monochromator nor pre-treating its spectra by orthogonalizing to spectral differences between the two instruments seriously damaged the predictive performance of the calibrations on Instrument 1. It was then possible to transfer these robust calibrations to Instrument 2 with a very simple correction for mean spectral difference and obtain acceptable results on prediction samples. Because Instrument 2 sees fewer samples, it was necessary to measure more replicates to match the performance of Instrument 1.

Characterization of maize silage with on-site NIRS sensors

Example 1

We used the NIRS instruments employed above and a total of 261 wet and intact maize silage samples.

To transfer the prediction models for dry matter, ash, crude protein, neutral detergent fiber and starch contents, digestibility of organic matter and fermentative parameters: pH, ammonia-N, lactic acid and volatile fatty acids, both instruments were standardized applying a standardization matrix developed with ten maize silages in order to adjust the differences between instrument wavelengths. The success of transference was evaluated by comparing the global and neighborhood average distances between on-site and at-line instruments before and after the standardization process. The external validation of the final calibration model was carried out by comparing reference versus predicted values using a mean comparison test (student-t). The results were satisfactory without significant differences between reference and NIRS with the exception of starch. These results have demonstrated the availability of NIRS technology to obtain nutritive and fermentative information of wet intact maize silages in real time outside the laboratory.

Example 2

More recently an innovative NIRS technology based on a combination of micro-electro-mechanical system (MEMS) and digital transform spectroscopy (DTS) has been employed to develop a portable spectrometer. This new device allows the compilation of spectra data in the labor field with high contrast pixelate.

To transfer the prediction models of nutritive parameters developed in an at-line instrument, using 241 wet and intact maize silage samples, different size standardization matrixes (from one to sixty samples), developed with the algorithm of Shenk and Westerhaus (1995), were tested. GH and NH values calculated with external validation sets were all reduced using the method with sixty standardization samples. 100 % of external samples giving GH values fewer than 3.0 (GH value 1.46). The best SEP results were obtained for dry matter, acid detergent fiber and starch contents (2.8; 0.6 and 2.4 %, respectively), with slightly higher accuracy than the models developed for at-line instruments.

These results suggest that the handheld MEMS-NIRS instrument, cheaper and easier for routine analysis, is suitable for in-situ applications. Nevertheless recorded measurements of spectra are critical due to the small sampling area. This requires increasing the number of spectra recorded for each sample to be representative of samples and using a high number of standardization samples to transfer a database from an at-line instrument to a MEMS- NIRS device in heterogeneous products such as maize silages.

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