STANDARDISATION OF NIR INSTRUMENTS, INFLUENCE OF THE CALIBRATION METHODS AND THE SIZE OF THE CLONING SET

PIERRE DARDENNE*[1], IAN A. COWE[2], PAOLO BERZAGHI[3,4], PETER C. FLINN[5], MARTIN LAGERHOLM[2], JOHN S. SHENK[6] and MARK O. WESTERHAUS[6]

[1] *Centre de Recherches Agronomiques de Gembloux – CRAGx, 24, Chaussée de Namur, 5030 Gembloux, Belgium.*
[2] *Foss Tecator AB, Box 70, SE-263 21 Höganäs, Sweden.*
[3] *University of Padova, Agripolis, 350020 Legnaro Italy.*
[4] *University of Wisconsin, 1925 Linden Dr., 53706 Madison, WI, USA.*
[5] *Agriculture Victoria, Pastoral and Veterinary Institute, Private Bag 105, Hamilton, Victoria 3300, Australia.*
[6] *Infrasoft International, 109 Sellers Lane, 16870 Port Matilda, PA , USA.*

A previous study (Berzaghi et al., 2001) evaluated the performance of 3 calibration methods, modified partial least squares (MPLS), local PLS (LOCAL) and artificial neural networks (ANN) on the prediction of the chemical composition of forages, using a large NIR database. The study used forage samples (n=25,977) from Australia, Europe (Belgium, Germany, Italy and Sweden) and North America (Canada and U.S.A) with reference values for moisture, crude protein and neutral detergent fibre content. The spectra of the samples were collected using 10 different Foss NIRSystems instruments, only some of which had been standardised to one master instrument. The aim of the present study was to evaluate the behaviour of these different calibration methods when predicting the same samples measured on different instruments.

Twenty-two sealed samples of different kind of forages were measured in duplicate on seven instruments (one master and six slaves). Three sets of near infrared spectra (1100 to 2500nm) were created. The first set consisted of the spectra in their original form (unstandardised); the second set was created using a single sample standardisation (Clone1); the third was created using a multiple sample procedure (Clone6). WinISI software (Infrasoft International Inc., Port Mathilda, PA, USA) was used to perform both types of standardisation. Clone1 is just a photometric offset between a "master" instrument and the "slave" instrument. Clone6 modifies both the X-axis through a wavelength adjustment and the Y-axis through a simple regression wavelength by wavelength. The Clone1 procedure used one sample spectrally close to the centre of the population. The six samples used in Clone 6 were selected to cover the range of spectral variation in the sample set. The remaining fifteen samples were used to evaluate the performances of the different models. The predicted values for dry matter, protein and neutral detergent fibre from the master instrument were considered as "reference Y values" when computing the statistics RMSEP, SEPC, R, Bias, Slope, mean GH (global Mahalanobis distance) and mean NH (neighbourhood Mahalanobis distance) for the 6 slave instruments.

From the results we conclude that i) all the calibration techniques gave satisfactory results after standardisation.
Without standardisation the predicted data from the slaves would have required slope and bias correction to produce acceptable statistics. ii) Standardisation reduced the errors for all calibration methods and parameters tested, reducing not only systematic biases but also random errors. iii) Standardisation removed slope effects that were significantly different from 1.0 in most of the cases. iv) Clone1 and Clone6 gave similar results except for NDF where Clone6 gave better RMSEP values than Clone1. v) GH and NH were reduced by half even with very large data sets including unstandardised spectra.