Near infrared 3rd party instrument networking

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Introduction

Instruments with compatible scanning ranges are being offered by different vendors. This increases the possibility that a laboratory or network of laboratories might have instruments, or want to have instruments from more than one instrument manufacturer under the same management. A product database is very expensive to develop and because instrument vendors do not recognise software from other sources, NIR users are often forced to stay with one manufacturer, even though they may prefer to use another manufacturer's instrument. The software operating both routine operation and prediction model development becomes the factor limiting the laboratories choice for hardware.

New programs have been developed to address this situation: a routine operation middleware program, Uscan, and universal calibration software, Ucal. The objective of this report was to test the software performance with three instruments: a Unity 2400 drawer instrument, a Unity 2500 rotating top window, and a NIRSystems 6500 transport. Uscan operates in the background of both factory routine operating systems, collects the spectrum, trims it, and predicts the samples with the Ucal prediction engine.

Materials and methods

Study 1a

Fifty flour samples were used for this study. Each sample was placed in a small ring cup and scanned by all three instruments. The spectra were collected and processed through the optimised partial least squares (OPLS) calibration program, Ucal, to develop the prediction equation.

Results and discussion

The small differences in calibration performances (Table 1) among the instruments were not considered to be of practical significance.

Having satisfied ourselves that all instruments had very similar calibration errors, we proceeded to the second objective of making the instruments alike in prediction.

Table 1. Comparison of the protein, ash, and moisture prediction errors among instruments.

Instrument	2400			2500			6500		
Constituent	Protein	Ash	Moist	Protein	Ash	Moist	Protein	Ash	Moist
SEC	0.20	0.01	0.06	0.17	0.02	0.03	0.19	0.01	0.05
SECV	0.22	0.02	0.14	0.21	0.03	0.11	0.20	0.02	0.08
RSQ	0.63	0.99	0.99	0.82	0.99	0.99	0.81	0.99	0.99

Materials and Methods

Study 1b

We arbitrarily chose the Unity 2500 instrument as the master and the other two instruments (U2400 and NIRS6500) as the satellite instruments. First we trimmed the U2500 and the NIR6500 to the U2400 scanning range because it was the smallest scanning range, and developed the trimmed U2500 equation.

We then used a procedure in Ucal (Trans) to transfer the spectra of the U2400 and the trimmed NIR6500 to the master U2500 instrument. We chose the same single sample from each of the trimmed files and the master file. A correction file was produced to make the U2400 and the NIR6500 similar to the master U2500. That correction file was applied to each of the samples in each database.

To make the calibration equations more repeatable across instruments, we created a MIN file (file to minimise unwanted variation during calibration). The MIN file was produced by combining the same 5 transfer samples with each instrument into a file. The new calibration was then developed with the U2500 database and the MIN file.

Results and discussion

Table 2 contains the results of the study.

Each numerical value in Table 2 was calculated as the average standard deviation of the predicted values of the 50 samples. The *SD* values under the (None) heading in Table 2 were generated with the three instrument files before any corrections were made. A major improvement in the constituent *SD* was made when the host instrument spectra were corrected with the Trans file, Table 2. In addition, adding the MIN file to the U2500 calibration improved the unexplained error among instruments even further, Table 2.

Table 2. The standard deviation of predicted values across the three instrument platforms.

Compare	None	Trans	Trans+MIN
Protein	0.777	0.105	0.040
ASH	0.212	0.031	0.020
Moisture	0.408	0.097	0.063

Table 3. The average standard deviation of predicted values for each sample across the three instrument platforms.

Compare	None	Trans	Trans+MIN
Protein	0.322	0.120	0.138
Fibre	2.813	0.387	0.338
Starch	10.916	0.700	0.557
ASH	3.345	0.255	0.195
NDF	7.136	0.465	0.458

Materials and methods

Study 2

This study evaluated the capability of making three other instrument platforms predict alike. Data and files were provided by Dr. Pierre Dardenne, Department Head: Quality of Agriculture Products Department, Walloon Agriculture Research Center, Chaussée de Namur, 24 5030 Gembloux (Belgium).

The instruments were a Unity 2500, a Bruker FT-NIR, and a NIRSystems 6500 all scanning from 1100–2498 nm. The master instrument was the U2500 and a whole plant maize spectral database of 200 samples was obtained from the NIRSystems 6500. The product database was transferred from the NIRS6500 to the trimmed U2500 with a single sample.

Results and discussion

Using the U2500 as the master, the difference plots of each host instrument against the master were very similar within each host instrument but different between host instruments. This demonstrates that each manufacturer produces consistent but slightly different spectra for the same sample; therefore, predicting the composition of 20 independent test samples without any spectral correction resulted in unacceptable agreement among the instrument platforms. This is shown as the average standard deviation (*SD*) of the predicted values for each sample across the 3 instrument platforms (None) in Table 3.

Applying a single sample Trans file to these two host instrument files made a major improvement in the *SD* of agreement among these 3 instruments. Likewise, applying a minimisation file to one half of the 20 transferred samples and validating it against the other half, provided additional reduction in the *SD* of agreement. Protein was a small exception in the last comparison.

Conclusion

In general, these two studies verify that the Uscan-Ucal software is able to support different NIR instrument platforms that have the same scanning range. The Transfer files of the host instruments

would be embedded in the Uscan program operating in the background of the host instrument manufacturer's routine operation program. The MIN file would be applied to a single product file producing the predicted results of each instrument in real-time. This new procedure will provide the capability for networking 3rd party instruments together under the same product database and prediction model. Other product databases and 3rd party instruments will be evaluated through this system to confirm these results.