CALIBRATION TRANSFER FROM DISPERSIVE INSTRUMENT TO HANDHELD POLYCHROMIX PHAZIR 1624

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Introduction

Foss NIRSystem

Dispersive monochromators have been widely used over the last 25 years to build large data sets in agriculture. On the other hand, new handheld instruments based on the MEMS (Micro Electro Mechanical System) technology are an attractive solution for on-site analysis in the food and feed sectors. The objective of this study carried out in collaboration with AUNIR Company (http://www.aunir.co.uk/) is to assess the potentiality of a calibration transfer from a Foss NIRSystem 5000 to a Polychromix Phazir 1624 instrument. The Polychromix Phazir 1624 is an handheld near-infrared (NIR) spectrometer active in the 1600 – 2400 nm range. It combines a DTS (digital transform spectrometer) engine, a reflectance probe, rechargeable batteries, integrated computer and LCD display and software into one unit that can be used remotely, such as in field or industrial applications.

Polychromix Phazir

Materiel and methods

A dataset of 7930 spectra of cereal flour has been analyzed for several years by AUNIR and CRA-W using a Foss NIRSystem 5000. PLS calibration models have been developed using reference values for the 5 properties selected for this study: moisture, water absorption, starch damage, protein and ash content. In order to transfer these equations from the dispersive instrument (slave) to the handheld spectrometer (master), 40 flour samples were measured with both instruments and analyzed with reference methods for the 5 criteria. Because the Polychromix Phazir 1624 instrument is working in the range of 1600-2400 nm with a non constant step, the first important modification is the interpolation of the 700 wavelengths (1100-2498 nm with a constant step of 2 nm) of the Foss NIRSystem 5000 instrument to the 100 wavelength of the Polychromix Phazir 1624 instrument (1600-2400 nm with a non constant step of around 8 nm) . After check of the interpolation performance, 7 outliers were removed. The 33 remaining samples were used for the standardization of the instruments. Figure 1 shows the Foss mean spectrum after interpolation of the 33 samples set. The second modification is the correction performed on the 33 Foss spectra by adding at each wavelength the difference between the value of the mean spectra of the standardization set measured with the Polychromix Phazir 1624 instrument and the mean spectra of the same file measured with the Foss NIRSystem 5000 instrument. Figure 2 shows differences between Phazir mean spectrum and Foss mean spectrum after interpolation of the 33 samples set. Figure 3 shows the 33 Foss spectra after standardisation against the 33 Phazir spectra. This interpolation and bias correction were also applied to the large Foss database. This data treatment was carried out under Matlab 7.5.0 (R2007b).

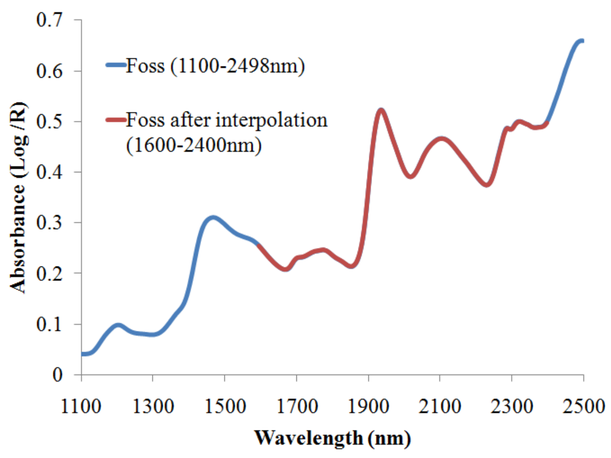

Figure 1: Comparison between Foss mean spectrum and Foss mean spectrum after interpolation of the standardisation set – 33 samples

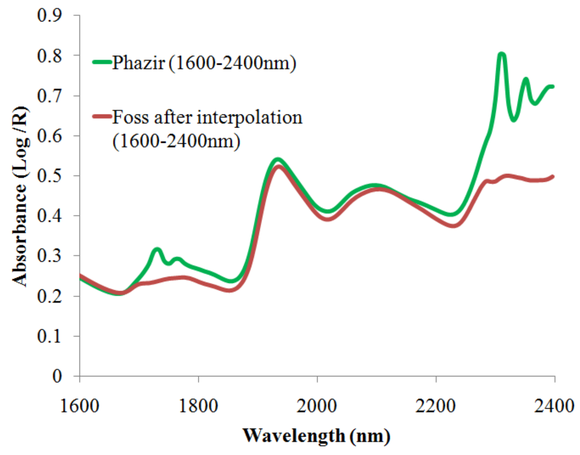

Figure 2: Comparison between Phazir mean spectrum and Foss mean spectrum after interpolation of the standardisation set – 33 samples

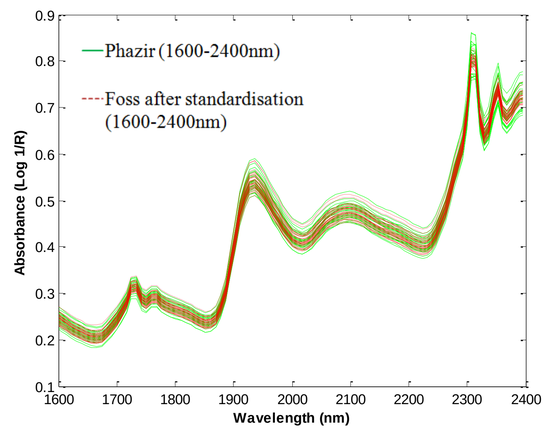

Figure 3: Comparison between Phazir spectra and Foss spectra after standardisation of the standardisation set – 33 samples

Results

Based on the spectral database of 7930 samples of cereal flour analyzed using a Foss NIRSystem 5000, different calibration models have been constructed, using reference values for moisture, water absorption, starch damage, protein and ash content. These models have been constructed using Partial Least Squares (PLS) as chemometric method and the results are summarized in Table 1. For each property, N represents the number of samples used to build the model, 'Min' and 'Max' represent the minimum and the maximum value respectively for that property, the fourth column indicates the number of PLS factors used and the last two columns show the root mean squared error when using leave-one-out cross-validation (RMSECV) and R^2 respectively.

Property	N*	Min	Max	Factors	RMSECV	R2
Moisture	1093	11.1	15.9	4	0.149	0.966
Water absorption	3387	47.0	73.8	11	0.913	0.942
Starch damage	882	2.0	45.0	11	2.547	0.846
Protein	1181	7.8	16.2	8	0.127	0.994
Ash	448	0.2	1.4	8	0.095	0.754

* The 33 samples of the standardization set (from the Foss instrument) have been added to the database

Table 1: Global models using the Foss NIRSystem 5000 full range (1100-2500 nm)

As previously explained, in order to transfer those equations from the Foss NIRSystem 5000 to the Polychromix Phazir, the set of 40 cereal flour samples analysed with both instruments was used for the standardization of the instruments. Seven outliers have been removed. Interpolation and bias correction were applied on the 33 remaining Foss spectra. From figure 3 it is clear that both instruments give similar spectra. Table 2 shows the transferred PLS models on the Polychromix Phazir instrument after standardisation and including the 33 samples of the standardisation set measured with the Polychromix Phazir instrument.

Property	N*	Min	Max	Factors	RMSECV	R2
Moisture	1093	11.1	15.9	5	0.170	0.955
Water absorption	3387	47.0	73.8	9	1.047	0.923
Starch damage	882	2.0	45.0	10	3.248	0.749
Protein	1181	7.8	16.2	7	0.316	0.964
Ash	448	0.2	1.4	8	0.114	0.644

* The 33 samples of the standardization set (from the Polychromix Phazir instrument) have been added to the database

Table 2: Transferred model to the Polychromix Phazir instrument (1600-2400 nm)

After the model has been transfer, it can be used for prediction of the samples included the standardization set. Table 3 shows the models parameters in prediction using the Foss NIRSystem (Model indicated in Table 1) and the Polychromix Phazir (transferred model indicated in Table 2) applied to the standardization set. The model parameters used for evaluation are the RMSEP (Root Mean Square Error in Prediction) and the R^2. The low R2 value for starch damage is linked to the low range of values for this property in the standardisation set compared to the full database.

Figure 4 : Prediction of flour parameters after calibration transfer on Phazir

					Foss model		Transferred model	
Property	N	Factors	Min	Max	RMSEP	R2	RMSEP	R2
Moisture	33	4/5	12.6	15.0	0.099	0.984	0.221	0.909
Water absorption	33	11/9	52.7	66.4	0.947	0.920	2.308	0.660
Starch damage	33	11/10	18.7	34.0	1.818	0.837	3.900	0.245
Protein	33	8/7	9.1	15.5	0.124	0.994	0.621	0.915
Ash	33	8	0.3	1.0	0.062	0.901	0.121	0.673

Table 3: Prediction using the Foss model and the transferred model on the standardization set

Conclusion

The achieved results show that calibration models for different properties of cereal flour developed on a Foss NIRSystem 5000 have been successfully transferred to a Polychromix Phazir 1624 handheld spectrometer, in particular for moisture and ash. Validation on external samples have to be performed.

References

Dardenne, P. (2004). Calibration Transfer in Near infrared spectroscopy. In: *Near Infrared Spectroscopy: Proceedings of the 11th International Conference, Davies, A.M.C. & Garrido-Varo, A. NIR Publications, 19-26.*

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