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EFFECT OF PORTABLE NIR INSTRUMENT AGEING ON FRUIT TSS PREDICTION

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ABSTRACT

There is a trend to take instrumentation from the laboratory to the field, e.g. spectrophotometers are commercially available for in field assessment of attributes of fruit on tree. Unfortunately, field users tend to place less emphasis on instrument maintenance, so understanding performance issues is important. Deterioration of lamp output quality over time and degradation of detector signal to noise ratio are issues associated with aging of an instrument. To document the effect of instrument aging on SWNIRS based fruit quality prediction, an experiment was conducted with several handheld PDA based spectrophotometers, with repeated spectra of a reference PFTE (Teflon) tile, and spectra of 20 apple fruit acquired at yearly intervals. Fruit total soluble solids (TSS) was also assessed, and used in development of a partial least squares regression (PLSR) models. The repeatability of each instrument was assessed as the standard deviation of absorbance of repeated measures of a reference, typically around 0.2 mAbs. Instrument changes were identified in performance and in PCA plots, but performance (apple TSS model) was not related to instrument repeatability.

KEYWORDS: apple, repeatability, partial least squares regression, spectrometer, total soluble solid

INTRODUCTION

Handheld diode array based SWNIR instruments are being used in field assessment of attributes of tree fruit. Sampling statistics dictate that for a population with a (typical) standard deviation of 1.5 % fruit total soluble solids (TSS) at 95% confidence interval with a margin of error of 0.2%, at least 225 fruit should be sampled, an application suited to a rapid non-destructive method such as NIRS. Unfortunately, field users tend to place less emphasis on instrument maintenance, so understanding of performance issues is important. The performance over time of a visible-shortwave near infrared spectrophotometer used in estimation of fruit attributes will depend on several factors, including aging of the light source, and ambient temperature of lamp and detector system.[1] Changes in the detector can include changes in relative spectral sensitivity, wavelength drift and degradation of detector signal to noise ratio. For example, Greensill et al.[2] demonstrated that for the application of assessment of sucrose concentration of aqueous solutions on cellulose fibre, model performance was decreased if wavelength resolution decreased beyond approximately 10 nm (FWHM) and repeatability decreased below approx. 0.1 mA (assessed as SD of repeated measures of a white reference, relative to that reference). Change in either detector or lamp response will impact the output of a predictive model of fruit attributes, primarily in terms of bias.[3, 4] However, while change in ambient temperature is known to affect halogen lamp output, but in practice spectral quality is not affected sufficiently to impact TSS model predictions, and ageing of a halogen lamp is also not associated with changes in light quality, at least until near lamp failure.[3, 5] Increasing temperature also affects silicon photodiode photo-response (becoming more sensitive to longer wavelengths), and also increases thermal noise.

Other instrument changes may also occur over time, affecting performance, e.g. probe alignment and wavelength. The effect of small (sub nm) change in wavelength calibration of a diode array unit can be very dramatic in terms performance of a TSS model. These authors reported that a drift of 0.03 nm over 150 days and 0.1 nm over a year period for Zeiss MMS1 diode array spectrometers. Instrument drift, as mentioned in a white paper from the NIR instrument manufacturer Foss (http://goo.gl/gwxa4C), is a well-established performance issue for NIR spectrometers.[6]

Model performance across years may thus be impacted by change in instrument characteristics. The objective of this study was to assess the impact of SWNIR instrument aging on spectral quality and its implication to apple predictive model performance over a period of several years.

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MATERIALS AND METHODS

The change in repeatability of three Nirvana handheld SWNIR spectrophotometers (Unit 05, 16 and 18) (Integrated Spectronics, Sydney; note this company is no longer trading, but the successor instrument F750 is available from Felix Instruments, Camas, USA) was assessed over three years, following periods of intensive field use each year. This instrumentation contains a Zeiss MMS1 spectrometer and a halogen lamp in a "shadow probe" interactance geometry[7]. Spectra (n=20) of a PTFE tile and from 24 ripened fruit, twice from each side, were collected once per year over three years. TSS was assessed of juice extracted from a tissue core to 1 cm depth from the same spot where spectra were collected, using a temperature compensated refractometer (Bellingham and Stanley RFM320).

Apple and PTFE white tile spectra were manipulated to produce interpolated (to 3 nm steps) absorbance and second derivative (Savitsky-Golay, second order, 4 data points each side) (id2A) spectra. Partial least squares regression (PLSR) models for TSS assessment were developed using mean centred second derivative absorbance data in the wavelength range 732-936 nm. These tasks were conducted using script written in Matlab2014a (MathWorks Inc., Natick, USA) using PLS toolbox 7.5.1 (Eigenvector Research Inc., Wenatchee, USA). Principle component analysis (PCA) was undertaken using The Unscrambler (v10.3, Camo, Norway). Full cross validation method was used for PLSR model cross validation.

RESULTS AND DISCUSSION

The spectra of the PTFE tile presents an absorbance 'feature' in the visible region. The instrumentation uses an internal gold plated shutter as an internal reference with every sample measured. Absorbance spectra of the PTFE (white) tile differed between instruments in the region 400-500 nm. This result is consistent with differences in the internal gold reference between units, with gold being a good reflector on infrared wavelengths, but absorbing in the visible region. The PTFE spectra also varied across years for unit 05, inferring change in the gold reference.

The standard deviation (SD) of 20 repeated PFTE absorbance spectra was used as a measure of instrument repeatability, with typical values for the region between 600 and 900 nm being less than 0.2 mAbs units (Table 1), comparable to the criterion (0.1 mAbs; above which model performance decreased) established for the Zeiss MMS1 module of for assessment of sucrose solutions on cellulose). Instrument repeatability was generally consistent over time (Table 1); however a poorer repeatability was recorded in 2010 for unit 5.

A PCA plot, weighted to wavelengths below 500 nm, of absorbance spectra of PFTE from three instruments over three years demonstrated spread with a given instrument in PC-1 (Figure 1). The spread in PC-2 between units was reduced in PCA plots of second derivative absorbance data, as expected for removal of baseline shifts in the absorbance spectra. The wavelengths loading for PC-2 also featured wavelengths below 500 nm. This is consistent with the observed difference in the white reference spectra for this unit. These differences between units and years are ascribed to differences in the gold coating of the reference shutter. PCA of second derivative absorbance apple spectra showed little spread between units and years.

Predictive model performance for apple TSS was comparable to other reports in the literature (e.g. typical RMSECV 0.6 %TSS). Whilst performance varied between years, this performance was neither correlated to unit repeatability nor was a trend with time apparent (Table 1). For example, in 2013 unit 16 produced an apple TSS model superior to the other two units, but recorded the poorest instrument repeatability (SD of 3.5 mA). Thus all units were operating with repeatability values (up to 3.5 mAbs) that were adequate to the task of apple TSS prediction.

Lu and McLure[8] reported that full spectrum calibration methods such as PLSR does surprisingly well in prediction of a three component mixture even with the presence of 99% noise (CV 0.17). They also reported that for PLSR of a natural product attribute (nicotine in tobacco), prediction error became poor only when noise was >30% (CV of 0.05). Thus while signal-to-noise ratio is important, its impact must investigated in context of an application. This conclusion is consistent with the observed poor relationship between white tile repeatability and apple model performance, at least for repeatability to 3.5 mAbs.

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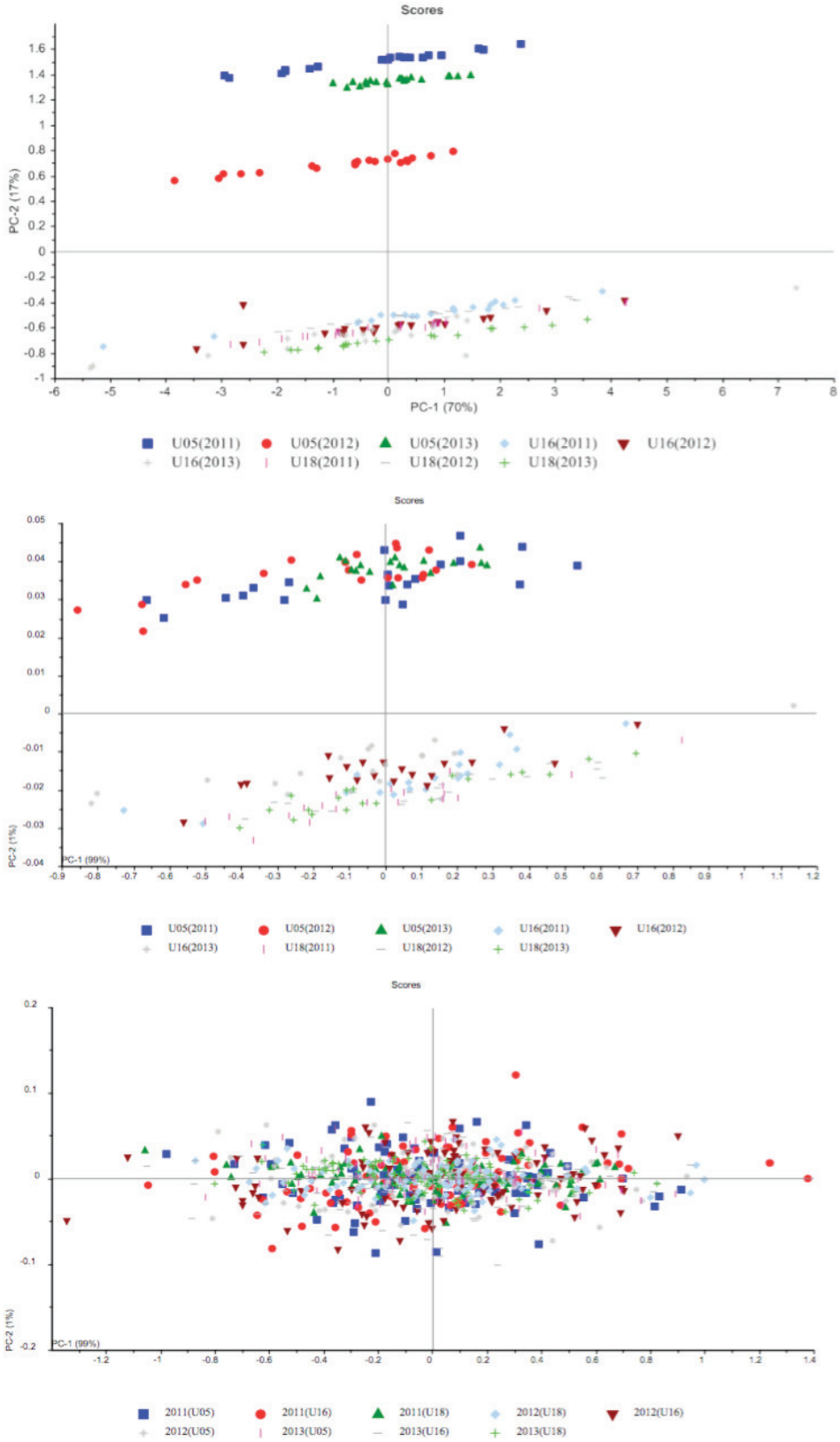

Figure 1. PCA score plot of (a) Absorbance white tile spectra, (b) D2A white tile spectra and (c) D2A apple spectra from three instruments over three years.

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Table 1. Table 1. Apple TSS model (based on id2A spectra over 729-975 nm) from three units over a time period of 3 years. Values in bold highlight the unit with best repeatability and apple model performance in each year. Apple TSS SD was 1.75, 1.53 and 1.51 in the years 2011, 2012 and 2013, respectively.

Year	Unit	White tile	SD PCs	R^2cv	RMSECV	SDR
2011	5	0.219	7	0.91	0.521	3.36
	16	0.613	7	0.87	0.625	2.80
	18	0.198	6	0.90	0.540	3.24
2012	5	0.185	9	0.79	0.713	2.15
	16	0.416	9	0.83	0.633	2.42
	18	0.256	8	0.84	0.608	2.52
2013	5	0.121	5	0.84	0.610	2.48
	16	3.523	5	0.82	0.640	2.36
	18	0.188	7	0.86	0.566	2.67
2011-12	5	-	8	0.85	0.636	2.59
	16	-	8	0.84	0.666	2.48
	18	-	8	0.88	0.564	2.93

CONCLUSION

No evidence for a consistent decrease in apple TSS calibration performance was found, indicating instruments were stable over the period of experimentation, despite extensive field use under tropical conditions. White tile repeatability varied between instruments and years but it was not a good indicator of apple model performance. Instrument updating with spectra collected over years had a satisfactory prediction within same instrument. The variation in units was mostly at the visible region, and attention should be given to stabilising the reference.

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