

Accurate Technique for Measuring Color Values of Grain and Grain Products Using a Visible-NIR Instrument

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ABSTRACT

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Measuring color is important when assessing grain and grain products as this has a major influence on the end-product quality. To objectively measure color, grain processors and plant breeding programs use colorimeters to measure $L^*a^*b^*$ values as defined by the Commission Internationale de L'Eclairage (CIE). In addition to color, most laboratories undertake other tests, often utilizing NIR (near infrared reflectance) technology. It is possible to improve laboratory efficiencies and remove double handling of samples by using one instrument, a visible-NIR spectrophotometer (400–2,500 nm), to measure color and other quality traits such as protein. In this study, we compared two techniques for measuring

color of flour, barley, and lentils with a visible-NIR instrument. The first technique involved calibrating the visible-NIR instrument with colorimeter values using calibration models. However, calibrations are product-specific and require the development and maintenance of specific equations for each product analyzed. For the second technique, we calculated the color values from the visible reflectance spectra using the standard practice (E308) based on the CIE system. Our study showed the most accurate, efficient method for measuring the color of products with a visible-NIR instrument is to apply calculations using the standard practice based on the CIE system.

The first quality evaluation a consumer makes on raw materials is a visual assessment that often includes the color of the product. This makes the color of grain and grain products an important trait for the food industry, as an acceptable color is often associated with freshness, cleanliness, and general product quality.

The relative importance and specific characteristics desired of grain or flour color varies with the product and market. For the flour industry, manufacturers of Japanese udon noodles prefer creamy colored flour (Mares and Campbell 2001), whereas manufacturers of pan bread specify flour with a bright white color. In the malting barley industry, maltsters require grain that is bright and free from staining because fungal stained or weather-damaged barley can cause cloudy and discolored beer. The lentil industry demands that red lentils, when split, should be a bright red-orange color. The seed color of lentils determines the consumers' decision to purchase the product and therefore directly affects marketability (Shahin and Symons 2003). As a result, grain handling companies, processing plants, and grain breeding companies routinely determine the color of wheat flour, whole grain barley, and whole grain lentils as a part of the quality assurance process.

There are numerous colorimeters and spectrophotometers available to objectively measure the color of raw materials or of a final product. These instruments can define the color in terms of CIE (Commission Internationale de l'Eclairage, ASTM 1996) L^* , a^* , and b^* values. These coordinates determine lightness (L^*) and chromaticity (a^* defines red/greenness and b^* defines yellow/blueness) of samples (Hunter 1975). Measuring color using CIE $L^*a^*b^*$ is widely accepted throughout the agricultural industry for assessing visual quality of products (Oliver et al 1992; Dowell 1998; Morris et al 2000; Garcia-Esteban et al 2003; Shahin and Symons 2003).

Colorimeters such as the Minolta chromameter measure illumination and reflected light filtered to detect the primary stimulus values for red, green, and blue light; these measurements are used to determine chromatic values such as the CIE $L^*a^*b^*$ coordinates. Another approach to measure the color of objects is to use the visible spectra reflectance data from a spectrophotometer and apply the same standard observer curves (E308) of the American Standards of Testing Materials (ASTM) based on the CIE system (Hunter 1975; ASTM 1996). CIE $L^*a^*b^*$ values are calculated by

using the spectral reflectance data for the object and applying the tables of standard values for the spectral tristimulus values (color matching functions) of a standard observer and spectral power distributions of a standard illuminant (ASTM 1996). This technique has been applied to data derived from color spectrophotometers to determine the color of objects such as soil (Mathieu et al 1998), ham (Garcia-Esteban et al 2003), flour (Oliver et al 1992), and grain (McCaig 2002). The advantage of applying these calculations to the spectra is the broad application to all products that can be scanned in a visible-NIR instrument.

An instrument that can be used to measure the color of a sample is a visible-NIR monochromator that measures the region from 400–2,500 nm. The use of NIR instruments is widely accepted throughout agricultural industries as a nondestructive secondary method for measuring various quality constituents of grain and flour. Such quality constituents include protein content, moisture content, hardness, oil content, starch properties, and fiber content (Delwiche et al 1998; Williams and Norris 2001).

Most grain handlers and researchers currently use NIR monochromator instruments by applying commercial calibrations or in-house calibrations, commonly using regression techniques such as partial least squares (PLS) or multiple linear regression (MLR) to build calibration models (McCaig et al 1993; Dowell 1998; Dardenne et al 2000). However, to develop these calibrations for new applications such as measuring color values requires calibration expertise, software tools to develop the equations, and a reference laboratory with qualified staff and equipment. In addition, calibrations need to be validated with target samples so that the ruggedness and precision of the calibration is maintained.

In this study, we compared two techniques to measure CIE $L^*a^*b^*$ color values of wheat flour, whole grain barley, and whole grain lentil samples using a visible-NIR instrument: 1) application of calibrations to estimate the color; and 2) calculating the color using the standard practice based on the CIE system. The advantage of using a visible-NIR instrument to reliably measure the color values of grain is that grain handlers can use this information to objectively classify and grade the color of a sample at the point of delivery in addition to simultaneously measuring the protein and moisture.

MATERIALS AND METHODS

Materials

In this study, two techniques for measuring color values (CIE $L^*a^*b^*$) from spectral data using a NIRSystems 6500 instrument were evaluated. The first technique assessed was the application

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of calibrations derived from the spectra and the laboratory reference data for estimating color values (Technique 1).

The second technique involved applying the standard practice based on the CIE system (Standard E308-95, ASTM 1996) for calculating color values from the spectra (Technique 2). These two techniques were compared with the reference method. The reference method involved obtaining color values from two colorimeters, one designed for measuring powders (Minolta CR200 colorimeter) and the other for measuring coarse material (Minolta CR310 colorimeter). The three instruments were standardized to minimize the differences arising from instrument geometry, optics, signal differences, lamp temperature, and power supply. Commercial tiles that had been matched to the Series II standard tiles (British Ceramic Research Association 1986) were used for the standardization.

Grain Samples

Cultivars of wheat, barley, and red lentils used in this study were grown at various sites throughout Australia in the states of Victoria, South Australia, and New South Wales in 2001 and 2002. All analyses were performed on clean grain, where the wheat and lentils were cleaned over a 2.0-mm screen and the barley was cleaned over a 2.2-mm screen. The wheat flour was produced by conditioning grain to 14.5% moisture and milled to straight run (Buhler Laboratory Mill Type MLU-202, Uzwil, Switzerland). In this study there were 346 flour samples, 324 barley samples, and 314 lentil samples used to develop NIR calibration models and for validation purposes.

Color Measurement Using Minolta Colorimeters

The CR-200 and the CR-310 chromameters (Minolta Camera Co., Osaka, Japan) were used to measure the color ($L^*a^*b^*$) of the flour and grain samples. These chromameters use a pulsed Xenon arc lamp filtered to match the CIE Standard Observer Response. The color meters have a viewing angle of 0° with the specular component included and are preset with the 2° observer; the C standard illuminant was selected for the purposes of this study. The CR-200 chromameter has an 8-mm diameter measuring area for accurate measurements of fine particulates tightly packed into a glass-surfaced cell such as flour. The CR-310 chromameter uses a wide area of illumination with a 50-mm diameter measuring area to average the reading over a wide area for measuring textured surfaces such as grain.

Wheat flour. The flour color ($L^*a^*b^*$) was measured using the CR200 colorimeter according to the Royal Australia Chemical Institute method 09-02 (RACI 2003). For uniform sample presentation, the flour was packed into a Technicon IAA near-infrared spectrophotometer (NIRS) cell (Bran and Luebbe, Norenstadt, Germany) (Oliver et al 1992). The measuring head of the CR200 colorimeter was carefully placed onto the center of the glass of the cell and a color measurement was taken. The flour sample was packed and measured once because the particle size is small and consistent due to the sieving process of milling, therefore the reproducibility error of sampling is low.

Whole grain barley. Whole grain color ($L^*a^*b^*$) was measured using the CR310 colorimeter. The barley grain was poured into a glass petri dish and scraped flat. The measuring head of a CR310 colorimeter was carefully placed into the petri dish and a color measurement was taken. The sample was repacked and measured for color three times to reduce the sampling error due to the irregularity of grain size. The three color values were averaged.

Whole grain lentils. The lentil color ($L^*a^*b^*$) was measured by pouring the grain into a plastic sample cup. The grain was settled and the measuring head of the CR310 colorimeter was carefully placed into the cup and a color measurement was taken. The sample was repacked and measured for color nine times to reduce the sampling error due to grain size irregularity and grain color variability of the lentils. The nine color values were averaged.

Color Measurement Using Visible-NIR Instrument

The flour and grain samples were equilibrated to 21°C in the NIR laboratory for 24 hr. The reflectance spectra, $\text{Log}(1/R)$, of the samples were recorded on a monochromator (model 6500, Foss NIRSystems, Silver Springs, MD) with a spectral range of 400–2,498 nm and 5-nm wavelength increments. Diffuse reflectance readings of an internal ceramic tile within the scanning module were referenced before and after the sample was scanned. The flour samples were packed in a spinning cup cell and measured through the automatic spinning cup module. The grain samples were packed in a standard coarse NIR sample cell and measured through the transport module.

Standardizing Measuring Instruments Using Reference Color Tiles

A set of ceramic color standard tiles (Series II) supplied by the British Ceramic Research Association (B Ceram RA, Stoke-On-Trent, England) were used to standardize the two colorimeters. The set consisted of three grey standards, seven chromatic standards (deep blue, red, deep pink, cyan, green, orange, and bright yellow), and two color difference standards (green and grey). The standard tiles were equilibrated to 21°C in the NIR laboratory for 24 hr. Each tile was measured for CIE $L^*a^*b^*$ on both the CR200 and the CR310 chromameter and the instruments were then matched using linear regression equations to the color values using the C illuminant, a 2° observer, and a geometry of $0^\circ/45^\circ$ (British Ceramic Research Association 1986).

Commercial tiles were used to standardize the visible reflectance data because the B Ceram RA Series II standard tiles were too large to fit in the scanning modules of the NIR instrument. The commercial tiles were tested for color uniformity by scanning nine times across the tile surface with the two colorimeters. The CIE $L^*a^*b^*$ values of each commercial tile were then matched to the B Ceram RA Series II standard tiles and averaged for both colorimeters. The commercial tiles were then cut to fit the NIR spinning cup cell without a quartz glass window front and glued into the cell. The tiles were then scanned in the NIR 6500 instrument transport module and the spinning cup module. The reflectance data from the NIR was then converted to CIE $L^*a^*b^*$ using the standard practice based on the CIE system (Standard E308-95, ASTM 1996) using the C illuminant, a 2° observer, and a geometry of $0^\circ/45^\circ$. The CIE $L^*a^*b^*$ values from the NIR instrument of the commercial tiles were matched to the previously averaged color values standardized from the CR200 and the CR310 instruments using linear regression equations, thereby standardizing all three instruments to the B Ceram RA Series II standard tiles.

NIR Prediction Models to Measure Color Values (Technique 1)

Three sets of NIR calibration models for CIE $L^*a^*b^*$ were developed on the 2001 and 2002 flour, barley, and lentil samples. The color data from both colorimeters were standardized to match to the B Ceram RA Series II standard tiles (British Ceramic Research Association 1986). The NIR calibrations for color values were formulated using software (WinISI II, v. 1.04, Infrasoft International, Silver Springs, MD). The mathematical criteria used to select samples for calibration development was the Mahalanobis distance or H statistic; samples that were within three H units for the population set were selected to develop the calibration. The calibration spectra were corrected for scatter with standard normal variance (SNV) and detrending to remove nonlinear relationships. The three calibration sets were developed after optimizing the mathematical treatment (2,5,5,1) of the visible raw spectra (400–780 nm every 5 nm) by using modified partial least squares (mPLS) regression method and cross-validation technique (Shenk and Westerhaus 1993).

A separate validation set from trials from different sites that were not used in the calibration set were used for the purpose of com-

paring the precision of the NIR calibration models to the colorimeter measurements.

Calculating Color Values Using Standard Practice (E308-95) Based on CIE System (Technique 2)

For the separate validation sets, the visible spectral reflectance data from 400–780 nm were used to calculate CIE $L^*a^*b^*$ using American Society for Testing and Materials (ASTM) Standard E308-95 tristimulus weighting factors and illuminant spectral power distribution tables (ASTM 1996).

The $\log(1/R)$ data was exported from WinISI software v. 1.04 into a text file and each data point was converted to reflectance values. CIE tristimulus values XYZ were then calculated by summing the tristimulus weighting factors at 400–780 nm for the C illuminant and the CIE 1931 (2°) Standard Observer, and the reflectance data (ASTM 1996).

$$X = k \sum_{\lambda=400}^{780} R(\lambda)S(\lambda)\bar{x}(\lambda)$$

$$Y = k \sum_{\lambda=400}^{780} R(\lambda)S(\lambda)\bar{y}(\lambda)$$

$$Z = k \sum_{\lambda=400}^{780} R(\lambda)S(\lambda)\bar{z}(\lambda)$$

$$k = 100 / \sum_{\lambda=400}^{780} S(\lambda)\bar{y}(\lambda)$$

where $R(\lambda)$ is reflectance data at 5-nm intervals; $S(\lambda)$ is relative spectral power of the CIE C illuminant; $\bar{x}(\lambda)$, $\bar{y}(\lambda)$, $\bar{z}(\lambda)$ are color-matching functions of the CIE 1931 (2°) Standard Observer; and k is the normalizing factor, where Y is equal to 100 for a perfect reflecting diffuser.

CIE $L^*a^*b^*$ color values were calculated using CIE XYZ.

$$L^* = 116 (Y/Y_N)^{1/3} - 16$$

$$a^* = [500 (X/X_N)^{1/3} - (Y/Y_N)^{1/3}]$$

$$b^* = [500 (Y/Y_N)^{1/3} - (Z/Z_N)^{1/3}]$$

X_N , Y_N , and Z_N are the tristimulus XYZ (C illuminant and CIE 2° Standard Observer) values of a perfect reflecting diffuser (determined by substituting $R(\lambda) = 1.0$ in the calculations for XYZ above). Furthermore, the normalizing constant, k , was defined such that $Y_N = 100$. Also, the above calculations for $L^*a^*b^*$ assumed that X/X_N , Y/Y_N , and $Z/Z_N > 0.008856$.

The calculated color values were standardized, as described earlier to match the B Ceram RA Series II standard tiles (British Ceramic Research Association 1986). These results were then compared with the standardized color data from the two colorimeters.

RESULTS

NIR Prediction Models to Measure Color Values (Technique 1)

Nine prediction models were developed to measure CIE $L^*a^*b^*$ on three products: wheat flour, wholegrain barley and wholegrain lentils. The validation results of Technique 1 (the application of NIR calibrations) versus the reference data for each calibration are presented in Table I and Fig. 1A–I.

Three statistical methods are the most meaningful for evaluating the efficiency of predicting constituents using reflectance data (Williams and Norris 2001): the coefficient of correlation, the bias, and the RPD, defined as the ratio of the standard deviation of the laboratory data to the standard error of prediction. For whole grain NIR analyses, an RPD value of 5–10 indicates that the calibration is adequate for quality control; an RPD value of 2.5–5

indicates that the calibration is sufficient for screening purposes; and an RPD value of 1.0 indicates that the calibration is not able to predict the constituent accurately (Williams and Sobering 1993; Delwiche et al 1998). In this study, the magnitude of the RPD value was used to assess the variability of the application of Techniques 1 and 2 (computation from CIE standard tables) to the reference method.

Flour CIE L^* and b^* values are the most important color components for assessing the visual quality of the milled product, whereas the relationship between CIE a^* and flour color quality is not clear. For the validation set, the linear relationships between the predicted flour color values (Technique 1) and the reference values for measuring CIE L^* and b^* were highly correlated (0.80 and 0.90, respectively). The comparisons of Technique 1 to the reference data for CIE L^* and b^* were associated with low standard errors (0.27 and 0.43) and small biases (0.12 and 0.21), indicating accurate estimations of the color values. The RPD values for the prediction models were 1.6–2.3 with low standard deviations in the laboratory data (0.44–0.96), indicating that the calibrations, while highly correlated, may be suitable only for broadly classifying samples and may be too variable for quality control.

Barley grain color (CIE b^* and a^*) and brightness (CIE L^*) are important traits in assessing grain quality, indicating the extent of bleaching and staining due to preharvest weather conditions. For barley, the correlation coefficients between Technique 1 and the reference method for CIE a^* and CIE b^* were high (0.99 and 0.94, respectively). When comparing the predicted and reference data for CIE a^* , the RPD value was relatively high (3.96) and the calibration was suitable for classifying grain samples and may even be applied to quality control processes. However, for CIE b^* the RPD value was smaller (1.90), therefore the calibration may only be appropriate for broadly classifying samples. However, the bias values associated with CIE a^* and b^* values were extremely high for the sample set (–3.04 and 1.30, respectively). The high bias in the validation set may be explained by differences in pedigree, site, and seasonal factors that affect the seed shape, appearance, and composition. This indicates that further validation work is required to determine the source of variation associated with NIR calibrations because there is a need to ascertain whether the calibration can be adjusted for bias for a new sample set. The relationship between Technique 1 and the reference data for barley brightness was poorly correlated (0.55), with an RPD of 1.17, indicating that the calibration is not predicting the reference values and is not appropriate for screening purposes (Fig. 1D).

The seed coat color of the red lentil samples in this study varied from light tan to dark green. The relationship between Technique 1 and the reference method for CIE $L^*a^*b^*$ values varied from moderately correlated for CIE L^* (0.73) to highly correlated for CIE a^* (0.92) and CIE b^* (0.88), with relatively high standard errors (>0.73) (Table I). The low RPD value for CIE L^* and CIE a^* values (1.3 and 1.6, respectively) indicate that the calibrations vary in their ability to determine the diverse range of lentil color values. The RPD value for measuring CIE b^* (1.99) was acceptable for screening purposes. Even though acceptable correlations and RPD values were obtained, the bias values between Technique 1 and the reference method for CIE $L^*a^*b^*$ values were very high for the lentil samples. Figure 1 (G–I) highlights which samples are contributing to the high bias values. These samples appear to be lighter (high CIE L^*) and have lower CIE a^* and CIE b^* values and are clearly spectrally different to the calibration samples. The lentil samples in the validation set were grown at a different site and contained samples that are genetically different from the calibration set, therefore the high bias values may be associated with the different genetic and environmental factors that affected the physical appearance of the seed. In addition, the lenticular shape of the seed may create spaces due to the angle at which the seed packs in the cup, causing light scattering and increasing the variation of the color predictions. The error associated with these bias

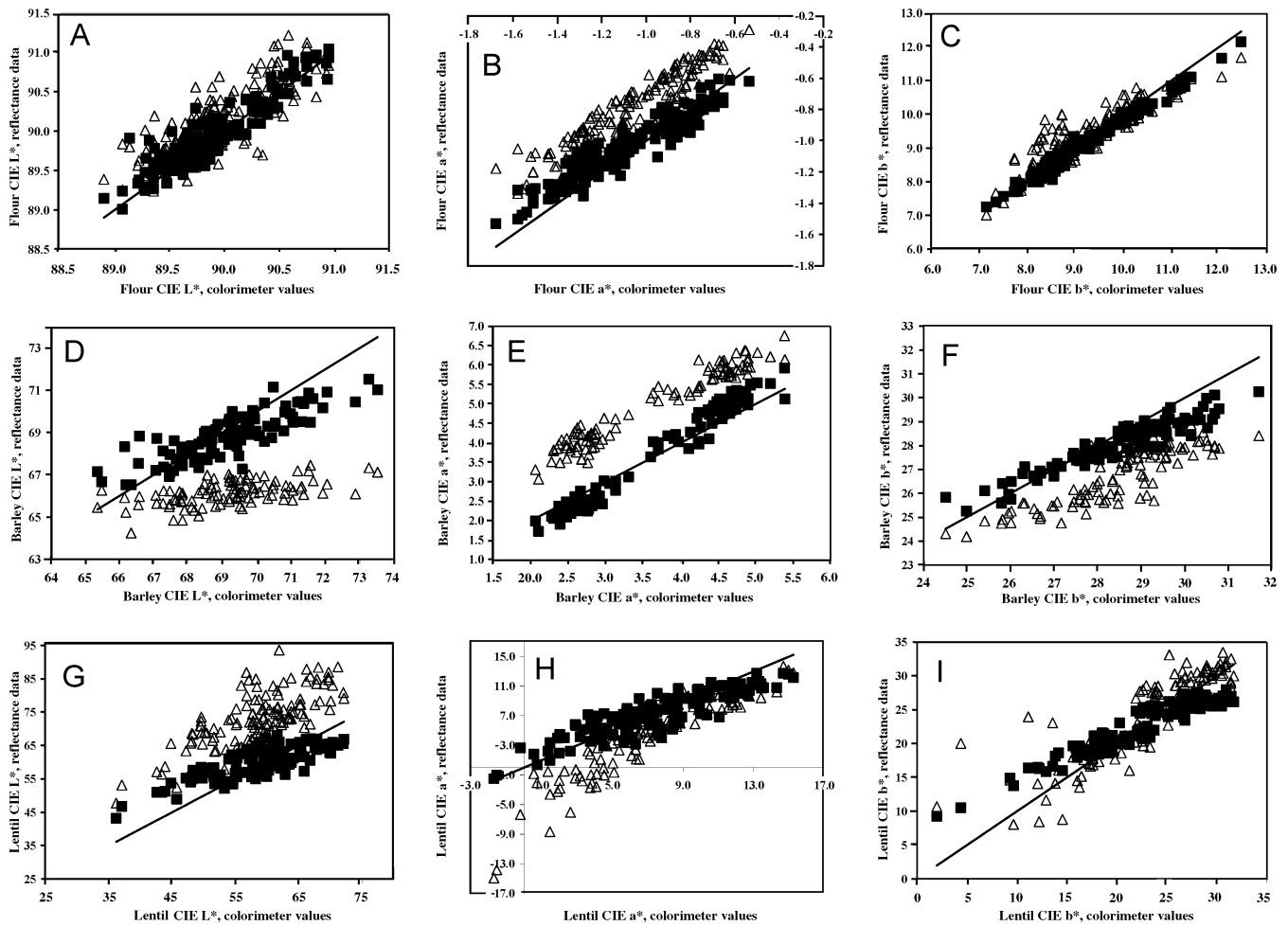


Fig. 1. Scatter plot of colorimeter reference CIE L*a*b* values plotted against the NIR predicted values (Δ) and against the calculated values based on the CIE system (\blacksquare), and a 1:1 line of best fit included. **A**, wheat flour brightness (CIE L*); **B**, wheat flour red-green (CIE a*); **C**, wheat flour blue-yellow (CIE b*); **D**, barley brightness (CIE L*); **E**, barley red-green (CIE a*); **F**, barley blue-yellow (CIE b*); **G**, lentil brightness (CIE L*); **H**, lentil red-green (CIE a*); **I**, lentil blue-yellow (CIE b*).

TABLE I
Validation Statistics for Measuring CIE L*a*b* Values Using Two Techniques

	CIE L*		CIE a*		CIE b*	
	NIR ^a	Calculation ^b	NIR	Calculation	NIR	Calculation
Flour (<i>n</i> = 166 validation samples)						
SDx ^c	0.44	0.44	0.24	0.24	0.96	0.96
<i>r</i> ^d	0.80	0.92	0.93	0.93	0.90	0.99
Bias ^e	0.21	0.05	0.27	0.05	0.12	-0.06
SE (C) ^f	0.27	0.17	0.09	0.09	0.43	0.16
RPD ^g	1.61	2.60	2.69	2.62	2.26	5.88
Barley (<i>n</i> = 103 validation samples)						
SDx	1.59	1.59	0.99	0.99	1.39	1.39
<i>r</i>	0.55	0.84	0.97	0.99	0.85	0.94
Bias	-3.04	-0.36	1.30	0.04	-1.72	-0.42
SE (C)	1.36	0.90	0.25	0.33	0.73	0.57
RPD	1.17	1.76	3.96	2.97	1.90	2.43
Lentils (<i>n</i> = 130 validation samples)						
SDx	7.15	7.15	3.69	3.69	5.98	5.98
<i>r</i>	0.73	0.78	0.92	0.88	0.88	0.95
Bias	14.39	1.14	-2.60	-0.25	1.17	0.02
SE (C)	5.66	4.58	2.30	1.76	3.01	2.69
RPD	1.26	1.56	1.60	2.09	1.99	2.22

^a NIR prediction data (Technique 1) applying calibrations derived from spectra and laboratory reference data for estimating color values.

^b Calculations based on CIE system (Technique 2) applying calculations using the standard practice based on the CIE system.

^c Standard deviation of the laboratory data.

^d Coefficient of correlation.

^e Average of differences between mean estimated value and reference value.

^f Standard error of estimated values corrected for bias.

^g Ratio of standard error to standard deviation of reference values.

changes would need to be quantified to determine whether NIR calibrations can be applied accurately to determine color values in lentils.

Calculating Color Values Using the Standard Practice Based on the CIE System (Technique 2)

Calculations to determine color values based on the standard practice (E308-95), Technique 2, were applied to the reflectance spectra for the same sets of wheat flour, whole grain barley, and whole grain lentil samples. Overall, there was an improvement in accuracy and precision by calculating CIE $L^*a^*b^*$ color values compared with that of the predicted values using NIR calibrations (Table I).

The relationships between Technique 2 and the reference method for measuring CIE $L^*a^*b^*$ color values on wheat flour were highly correlated (0.92–0.99), with equal or lower standard errors (SE < 0.17) than Technique 1. The accuracy of calculating the color values using Technique 2 were higher, as RPD values increased for CIE L^* and CIE b^* (2.60 and 5.88, respectively). This indicates that the accuracy in applying Technique 2 when measuring CIE L^* and CIE b^* may be more reliable than Technique 1 for screening and quality control purposes.

For barley grain, moderate to high correlations were observed between Technique 2 and the reference method (0.84–0.99), associated with similar or lower standard errors (SE 0.33–0.90). The low bias (–0.36) and moderate to low RPD value for CIE L^* (1.76) indicate that this technique may be sufficiently accurate for screening samples for barley brightness. CIE a^* and CIE b^* values from Technique 2 can also be used to classify samples into color groups as the RPD values were moderately high (2.97 and 2.43, respectively). However, Technique 2 tended to overcalculate CIE L^* and CIE b^* for the lower values and undercalculate for the higher values (Fig. 1D and F); the reverse was observed with CIE a^* values. This suggests that the application of linear regression for standardizing the spectrophotometer to the colorimeters may not be the ideal method.

For the lentil samples, the relationships between Technique 2 and the reference data for CIE $L^*a^*b^*$ were moderately to highly correlated (0.78–0.95) and associated with moderate errors (Table I). A phenomenon was observed with the whole grain lentil samples that was similar to that observed with the barley calculated values, this is most likely due to the limitations of applying the standardization method used in this study to whole grain samples. The RPD values for color were between 1.56 and 2.22, indicating Technique 2 may be sufficient for screening samples.

DISCUSSION

Spectrophotometers measure the physical properties of the light reflected by an object; colorimeters measure the psychophysical properties of an object and are designed to give measurements that correlate with the human eye-brain impressions. When developing alternate methods for measuring color, such as using a spectrophotometer, they need to be characterized with respect to other color instruments. Standardizing color instruments requires independent CIE $L^*a^*b^*$ values that define the appearance of a sample under a specified viewing illuminant of a standard observer. The standardization method used in this study was to apply linear regression using spectra collected from standard tiles. There are other procedures for standardizing spectrophotometers that estimate the differences in nonlinear spectral relationships (Fearn 2001; Shi and Healey 2002). However, these methods rely on complex mathematical algorithms. For the purpose of ranking samples, we concluded that linear regression was adequate for standardizing the three instruments when applied to wheat flour.

A simple standardization method such as the linear regression technique used in this study does not account for the many differences between the colorimeter and the spectrophotometer for the sample cups and sample types presented. Samples of grain (barley

and lentils) create spaces in the surface packing of the NIR cell, and thus much of the incident light is absorbed into the sample-packing matrix. Consequently, further work is required to develop standardization models that account for differences in the packing surface and the effects of metamerism, whereby the color appearance of two samples may rank the same when measured by a colorimeter but rank differently when measured by a spectrophotometer. Therefore, more samples of a similar color from many sites would need to be scanned on the colorimeter and spectrophotometer to explain the possible source of error.

The spectrophotometer was not specifically designed to measure the color of samples and the silicone detector does not have the photometric accuracy and precision of a colorimeter (Hunter 1975). However, many researchers have developed NIR calibrations for color to classify grain samples (McCaig et al 1993; Shenk and Westerhaus 1993; Dowell 1998). There are many requirements needed to develop NIR calibrations. These include expertise in NIR calibration software; analytical analyses of the products; sample diversity to include genetic differences and environmental conditions; and calibration development procedures (Williams and Cordeiro 1985; Shenk and Westerhaus 1993). As Technique 1 is a secondary method, any of these factors can limit the application of the calibrations. Spectrophotometers measure the physical properties of a sample, and complex NIR calibrations may confound the spectral properties during data treatment by removing the effects of particle size that affect the color appearance of a sample.

Technique 1 requires continuous development to ensure that the calibrations are predicting with the appropriate accuracy and precision, as new samples may differ due to varietal and seasonal factors that affect the seed coat appearance and seed composition. For a new set of samples, there may be a requirement to develop new calibrations to accurately predict color, requiring additional resources.

Our study has shown that the most reliable, cost-effective method for measuring the color of wheat flour, barley, and lentil with a visible-NIR spectrophotometer is Technique 2 by applying calculations based on the CIE system. The advantage of applying this technique is that the CIE tables are applicable for all products. The reflectance data, once standardized, simply need to be worked through the calculations as supplied by the CIE tables (E308) using the appropriate observer and spectral power distribution constants to determine CIE $L^*a^*b^*$ values. In addition, applying the CIE method eliminates the need to further process new samples through the laboratory to validate the method, as is constantly required when monitoring NIR calibrations. This also reduces costs.

The more accurate and reliable method to measure the color values of flour and grain samples using a visible-NIR instrument is Technique 2, when comparing the reference data to the two techniques. Higher correlations were observed for Technique 2, with reduced standard errors. The RPD values verified that the calculations based on the CIE system were suitable for applications other than merely grouping the samples. Technique 2 may, with improved instrument standardization, be applied to such applications in the food and grain industry for product quality control and grain classification.

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