Near-infrared Spectrometric Method for Nondestructive Determination of Soluble Solids Content of Peaches

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ABSTRACT. A nondestructive method for measuring the soluble solids (SS) content of peaches [*Prunus persica* (L.) Batsch] was developed using near-infrared (NIR) spectrometry. NIR transmittance in the 800 to 1050 nm region was measured for four cultivars of peaches ('Blake', 'Encore', 'Red Haven', and 'Winblo'), over a period of three seasons (1993 through 1995). Each fruit was scanned on both halves keeping the suture away from the incident light beam. Soluble solids contents of flesh samples taken from corresponding scanned areas were determined using a refractometer. Multiple linear regression models using two wavelengths were developed with second derivative spectral data and laboratory measurements of SS content. Multiple correlation coefficients (*R*) for individual cultivar calibrations within a single season ranged from 0.76 to 0.98 with standard error of calibration (SEC) values from 0.35% to 1.22%. Selected spectra and corresponding SS data in individual cultivar calibration data sets were combined to create season and cultivar calibration data sets to cover the entire range of SS contents within the season or within the cultivar. These combined calibrations resulted in *R* values of 0.92 to 0.97 with SEC values ranging from 0.37% to 0.79%. Simple correlations of validations (*r*) ranged from 0.20 to 0.94 and the standard error of prediction (SEP) ranged from 0.49% to 1.63% while the bias varied from -0.01% to -2.62%. Lower *r* values and higher SEP and bias values resulted when individual cultivar calibrations were used to predict SS levels in other cultivar validation data sets. Cultivar calibrations, season calibrations and the overall calibration predicted SS content of all validation data sets with a smaller bias and SEP and with higher *r* values. These results indicate that NIR spectrometry is suitable for rapid nondestructive determination of SS in peaches. Feasible applications of the method include packinghouse sorting of peaches for sweetness and parent and progeny fruit quality assessment in peach breeding programs. Using this technique fruit may be sorted into two or three sweetness classes. The technique may also potentially be extended to other fruit.

Due to the inherent variability in quality among individual units of fruit and vegetables, rapid nondestructive instrumental techniques for quality evaluation and assurance would be highly desirable. Nondestructive quality measurements do not damage or alter the product, hence the product can be marketed or used for other measurements. A wide spectrum of methods (e.g., light reflectance and transmittance, delayed light emission, fluorescence, nuclear magnetic resonance, acoustic response, dielectric response, force deformation, impulse force response and X-ray) have been tested for the measurement of a range of quality attributes in fruit and vegetables [American Society for Agricultural Engineering (ASAE), 1994; Chen and Sun, 1991; Dull, 1986].

Infrared spectrometry is currently a widely used technique for food and agricultural analyses, with most applications involving the near-infrared (NIR) region (700 to 2500 nm) (Wilson, 1995). The NIR region has been exploited due in part to the availability of strong radiation sources and detectors with high sensitivity. Thus the signal-to-noise ratio of measurements is generally higher and/or individual samples can be assessed much more quickly than, for example, the midinfrared (MIR) region (2500 to 25000 nm), though the latter contains potentially valuable analytical information (Carrol, 1995). A higher signal to noise ratio in the NIR region allows for the use of a longer light path, thus giving a more sensitive measurement. As a consequence, NIR spectrometry has been used in the nondestructive quality evaluation of a variety of fresh fruit and vegetables (ASAE, 1994; Dull, 1986). Applications

range from sensing external quality attributes such as surface defects (Throop et al., 1992; Upchurch et al., 1990a) to many internal characteristics such as moisture content (Dull et al., 1991), dry matter (Birth et al., 1985; Dull et al., 1989), sugars (Kawano et al., 1992; Slaughter, 1995) and soluble solids (Dull et al., 1992; Peiris et al., 1997).

Surface appearance and internal composition are critical considerations in assessing the quality of peaches. Though market acceptance of fresh peaches is based to a large extent on surface appearance, satisfaction and subsequent purchases depend on eating quality (Kader and Mitchell, 1989). Internal characteristics such as sugar content, soluble solids (SS), percentage titratable acidity, total solids, and soluble solids/acid ratio have been shown to be good indices of eating quality of peach (Sistrunk, 1985). Sugars comprise the major component of the SS in fruit juices. Among other soluble materials are organic and amino acids, and soluble pectins. Sugar content can be measured directly via chemical analysis, however, since sugars are usually the major component of soluble solids, it is much easier to simply measure total SS in extracted juice with a refractometer (Wills et al., 1989). Both methods, however, are destructive.

According to national consumer surveys, peaches were considered as the least consistent in quality by 40% of consumers in 1988 and 1989 and consumers were willing to pay 5 to 20 cents more per pound for high quality tree-ripe peaches (Bruhn et al., 1991). Hedonic analysis of peach prices has also shown that at the retail level fruit SS content significantly influences price. High SS can increase the price by more than \$2 per 8.6- to 10-kg box (Parker et al., 1991; Parker and Zilberman, 1993). Due to the lack of a technique to directly measure internal quality characteristics, the peach industry may be losing potential revenue by not fully capitalizing on the consumer's preference for high SS. As a

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consequence, it is important to incorporate internal quality characteristics into grading standards. To achieve this, new technologies are needed that allow the accurate, nondestructive measurement of SS and other flavor-related traits.

Nondestructive optical methods using light transmission (Sidwell et al., 1961) or reflectance (Romani et al., 1962; Bittner and Norris, 1968; Upchurch et al., 1990b) have been tested as a means of grading peaches into maturity classes. The methods are based on measuring color which is correlated to maturity of fruit. Initial attempts to directly measure internal quality characteristics of peaches using nondestructive techniques indicated that the SS of peaches and nectarines may be measured using NIR techniques. Bellon et al. (1993) using a diode array NIR spectrometer showed that peach could be sorted into three groups based on SS with a reliability of 76%. Using a commercial NIR spectrometer equipped with a fiber optic probe, Slaughter (1995) demonstrated a relationship between NIR absorption and SS in peaches and nectarines. The calibration used four cultivars of peach and three of nectarine. Subsequently, Peiris et al., (1997) showed that SS in peach cv 'Blake' could be measured with a high level of accuracy and precision using an acousto-optic spectrometer. Over three consecutive growing seasons, multiple correlation coefficients for calibrations ranged from 0.91 to 0.98 and SEC values ranged from 0.42% to 0.52%. Calibrations developed for individual seasons, however, were less accurate in predicting SS of other seasons. A combined calibration using the spectral data of all three seasons showed a marked improvement in prediction performance, possibly due to the broader constituent range. However, the effects of different cultivars on a calibration as well as the effects of one cultivar's calibration on the validation of other cultivars were not investigated in these studies. It is hoped that the incorporation of additional cultivars could further improve the performance of calibrations. As a consequence, we report the NIR spectrometric analysis of the SS of four peach cultivars over three seasons.

Materials and Methods

Fruit of four peach cultivars ['Blake' (BL), 'Encore' (EN), 'Red Haven' (RH), and 'Winblo' (WB)] were used in the study over a period of three seasons, 1993 through 1995. Individual fruit were hand harvested at The University of Georgia Horticulture Research Farm, Athens, Ga., in the morning of each testing date. Immediately after harvest the fruit were brought to the laboratory, sorted to remove any defective (e.g., bruised, insect or disease damaged) fruit, brushed to remove fuzz that interferes with the optics of the instrument, weighed, and numerically coded. Harvest of each cultivar began before the initial color break and continued through the tree-ripe stage, obtaining the maximum possible range in SS content for each cultivar. Number of fruit scanned varied (Table 1) depending on the time and resources availability. Our objective was to scan as much fruit as possible to obtain the maximum possible range in SS content in each season. A small predetermined number of fruit for this kind of experiment often do not cover the entire range of SS content in a single cultivar.

An acousto-optic spectrometer (Jaenisch et al., 1990) was used to obtain the optical density spectra of intact fruit in the 800- to 1050-nm range at 0.5-nm intervals. An average of ten scans was used for final optical density spectra of each fruit. The spectrometer wavelength range to scan, interval between two wavelengths, and the number of scans to average for the final spectra were controlled by computer using a software program written in BASIC.

The reference optical density spectra were taken with a 25-mm-

thick Teflon disk. Fruit were placed in the instrument stem end down, keeping the suture away from the incident light beam for the first spectra, while the second spectra had the stem end up with the suture again oriented away from the light beam. Thus, two spectra (each an average of 10 scans) were collected per fruit, one on each half of the fruit. The detector was positioned at a 45° angle to the incident light beam and was tightly fitted to the fruit (or Teflon standard) using a rubber sleeve fitted around the detector such that stray radiation could not reach the detector while scanning. All scans were taken with the fruit sample enclosed within a black metal box during scanning.

After scanning, the SS content of each fruit was determined using a refractometer (ABBE-3L, Bausch and Lomb, Rochester, N.Y.). A flesh sample was obtained from the scanned area using a 10-mm cork borer and crushed using a garlic press to obtain a juice sample for measurement.

Soluble solids data were merged with the respective spectral data using Near-infrared Spectral Analysis Software (NSAS) program (NIRSystems, Silver Spring, Md.). A master data file was made for each cultivar separately for each season by merging all spectral and constituent data collected throughout the season for the cultivar. The file served as the source of spectra for calibration and validation data sets for the respective cultivars in each season. The spectra for each cultivar's master calibration file in a single season were then sorted by SS content and divided into strata of 0.50% SS levels. Nearly equal numbers of spectra were randomly picked from each stratum such that 60 spectra were selected to uniformly represent the entire SS range of the particular cultivar within the season for the individual cultivar calibration (i.e., the calibration of a single cultivar within a single season).

Twelve individual cultivar calibration regression models [i.e., BL calibration file for 1993 (BLC93) through WB calibration file for 1995 (WBC95)], were developed (one per cultivar per season) using the calibration data sets so that the final calibration had nearly 50 spectra after removing outliers or extreme observations (Rousseeuw and Leroy, 1987) during the regression model building. Four cultivar calibrations, [i.e., calibrations covering a single cultivar over three seasons (BLC, ENC, RHC, and WBC)] were made by combining selected spectral and constituent data of a particular cultivar over the three seasons. Likewise, three season calibrations or those covering all four cultivars within a single season (PC93, PC94, and PC95) were made selecting spectra from each of the four cultivar calibration data sets within a single season. Finally, an overall calibration for peach (PC) was made to represent spectra coming from all four cultivars and all three seasons. For the above mentioned combined calibrations, spectra were selected from appropriate individual cultivar calibration data sets developed for each cultivar in each season such that the selected spectra uniformly covered the full range of SS content observed in each season for each cultivar. For cultivar calibrations, 21 spectra (1, 4, 7, 10...60) were selected from each of the three season's individual cultivar calibration data sets so that the cultivar calibration data set for a particular cultivar had 63 spectra. Likewise, for season calibrations, 16 spectra (1, 5, 9, 13,...60) were selected from each of the four cultivar's individual cultivar calibration data sets within a single season. For the overall calibration, six spectra (1, 12, 24, 36, 48, and 60) were selected from each of the 12 individual cultivar calibration data sets. Selection of spectra in the above mentioned manner from the individual cultivar data sets allowed covering the entire range of soluble solids content obtained in each season for each cultivar as well as providing an equal number of spectra from each cultivar and each season in the combined calibrations.

The spectral data of the calibration data sets were converted to second derivative spectra with a segment size of 5 nm and gap size of 0 nm using the NSAS program. Finally, the second derivative spectral data were used to develop multiple linear regression models by linear combinations using two wavelengths. Fruit soluble solids content was modeled to second derivative optical density by $SS = K_0 + K_1 \times WL_1 + K_2 \times WL_2$, where, SS = soluble solids content of fruit (%), WL_1 = second derivative optical density at the first wavelength, and WL_2 = second derivative optical density at the second wavelength.

Each master validation file was sorted by SS content and 50 spectra were selected in the same manner as the individual cultivar calibration data sets to cover the entire range of SS content for the individual cultivar validation file for each season (i.e., BLV93 through WBV95). Four cultivar validation files (BLV, ENV, RHV, and WBV) each having 150 spectra were created merging all the spectral and constituent data of three individual cultivar validation files of each cultivar over three seasons. Three season validation files (PV93, PV94, and PV95) were made by merging the individual cultivar validation files of the four cultivars within a single season giving a total of 200 spectra. An overall validation file (PV), which had a total of 600 spectra was created by combining all twelve individual cultivar validation files. The fitness of the individual cultivar calibrations and the season calibration for each season was evaluated by predicting the SS contents of the respective individual cultivar and season validation data sets in all possible combinations separately for three seasons. Every season calibration and overall calibration was also tested by predicting SS contents of all season validations and the overall validation. All of the cultivar calibrations together with the overall calibration were also evaluated by predicting constituents in cultivar validations. Multiple correlation coefficient of calibration (*R*) and standard error of calibration (SEC) were used to evaluate calibration models while standard error of prediction (SEP), bias and simple correlation between actual and predicted constituent values (*r*) in validation data sets were used to test the applicability of calibrations.

Results and Discussion

The refractometer SS statistics for peach cultivars in each season and that found in all calibration models developed and validation data sets are given in Table 1. The SS content of fruit tested during the 3-year period of this study varied from 5.3% to 21.2%. 'Encore' had the highest mean SS content (14.4%) in 1995 while 'Red Haven' had the lowest (8.4%) in 1994. Late cultivars 'Encore' and 'Blake' had higher mean SS contents compared to that found in 'Red Haven' and 'Winblo' which are early cultivars. 'Encore' also had the highest range of SS content (13.5%) in 1993 while the same cultivar had the lowest range (3.4%) in 1994. 'Blake' had the highest variability in SS content in 1993 with a standard deviation of 1.65% while 'Encore' had the lowest variability in 1994 with a standard deviation of 0.77%. Some individual cultivar calibrations had lower ranges of SS because lower or upper end SS values were found to be outliers during regression model building. However, the variability of constituent data in calibration data sets was generally increased compared to the respective master data file as evidenced by higher standard deviations. This was due to the selection of spectra to cover the entire range of SS data uniformly.

The maximum, minimum and average optical density spectra (log 1/Transmittance) of peaches tested in 1995 from 800 to 1000 nm are shown in Fig. 1. The second derivatives of the three spectra given in Fig. 1 is shown in the 800 to 940 nm region in Fig. 2. The

Table 1. Soluble solids content (SSC) statistics for calibration and validation data sets.

Spectra		SSC (%)				
	(no.)	Min	Max	Range	Mean	SD
Cultivar ^a						
BL93	320	8.8	21.2	12.4	12.0	1.65
BL94	166	6.8	13.2	6.4	9.6	1.22
BL95	390	10.0	16.5	6.5	12.7	0.92
EN93	298	6.0	19.5	13.5	12.2	1.45
EN94	246	8.8	12.5	3.4	10.9	0.77
EN95	300	10.0	19.0	9.0	14.4	1.11
RH93	288	7.8	13.7	5.9	10.3	1.17
RH94	158	5.8	10.8	5.0	8.4	0.98
RH95	122	6.7	12.5	5.8	9.8	1.31
WB93	288	6.0	15.8	9.8	11.8	1.58
WB94	144	5.3	12.0	6.7	8.6	1.43
WB95	382	5.4	13.3	7.9	8.5	1.39
Calibration						
BLC93	48	8.8	21.2	12.4	12.8	2.41
BLC94	54	7.2	11.8	4.6	9.5	1.10
BLC95	50	10.6	15.7	5.1	13.0	1.11
ENC93	48	9.9	16.2	6.3	12.7	1.69
ENC94	53	9.4	12.5	3.1	10.7	0.80
ENC95	54	12.4	18.3	5.9	14.4	1.15
RHC93	59	8.0	13.2	5.2	10.3	1.32
RHC94	57	6.2	10.7	4.5	8.4	1.08
RHC95	57	7.8	12.5	4.7	10.0	1.24
WBC93	58	7.0	15.0	8.0	11.4	1.98
WBC94	57	5.4	12.0	6.6	8.5	1.51
WBC95	50	6.0	13.3	7.3	8.8	1.71
BLC	51	7.2	21.2	14.0	11.6	2.55
ENC	55	8.8	18.3	9.5	12.5	2.06
RHC	47	6.2	13.2	7.0	9.5	1.57
WBC	49	5.4	15.8	10.4	9.6	2.35
PC93	50	8.0	21.2	13.2	12.1	2.29
PC94	56	5.4	12.5	7.1	9.2	1.67
PC95	56	6.7	19.0	12.3	11.7	2.63
PC	62	6.2	16.0	9.8	10.8	2.33
Validation						
BLV93	50	9.0	18.6	9.6	12.0	1.58
BLV94	50	6.8	12.2	5.4	9.7	1.27
BLV95	50	10.5	15.1	4.6	12.6	0.82
ENV93	50	7.2	19.0	11.8	12.1	1.67
ENV94	50	9.0	12.5	3.5	10.8	0.85
ENV95	50	10.0	17.2	7.2	14.3	1.18
RHV93	50	7.8	13.7	5.9	10.4	1.32
RHV94	50	5.8	10.8	5.0	8.6	1.01
RHV95	50	7.2	12.0	4.8	9.7	1.30
WBV93	50	6.0	15.2	9.2	11.9	1.70
WBV94	50	5.3	12.0	6.7	8.6	1.62
WBV95	50	6.0	13.3	7.3	9.0	1.91
BLV	150	6.8	18.6	11.8	11.4	1.79
ENV	150	7.2	19.0	11.8	12.4	1.92
RHV	150	5.8	13.7	7.9	9.6	1.41
WBV	150	5.4	15.8	10.4	9.6	2.35
PV93	200	6.0	19.0	13.0	11.6	1.72
PV94	200	5.3	12.5	7.2	9.4	1.52
PV95	200	6.0	17.2	11.2	11.4	2.56
PV	600	5.3	19.0	13.7	10.8	2.21

^aBL = 'Blake'; EN = 'Encore'; RH = 'Red Haven'; WB = 'Winblo'; V = a validation data set; C = a calibration data set; P = pooled (combined) data sets. The numerical designation indicates the production year (e.g., 93 = 1993). Therefore, BLC93 = 'Blake' calibration data set for 1993; BLV = 'Blake' validation set for all 3 years; PV = pooled validation set (all cultivars and years).

Fig. 1. Minimum, maximum and average near infrared diffuse transmittance spectra of peaches.

Fig. 3. Near infrared diffuse transmittance spectra of peaches with high and low soluble solids (SS) levels.

Fig. 2. Second derivative spectra of the minimum, maximum and average near infrared diffuse transmittance spectra of peaches from Fig. 1.

Fig. 4. Second derivative of the near infrared diffuse transmittance spectra of peaches (from Fig. 3) with high and low soluble solids levels.

optical density is dependent upon the length of the light path and the optical characteristics of the sample in the light path. Therefore, large baseline variations can be observed in optical density spectra as shown in Fig. 1. Our data with a total of 1194 spectra in 1995 showed a baseline shift of as much as 1.033 OD units at 800 nm. Likewise, 1194 spectra recorded in 1993 had a baseline shift of 0.883 OD units while 714 spectra taken in 1994 had a baseline shift of 0.813 OD units at 800 nm. Optical density spectra of two fruit, one with a low (6.7%) and the other with a high (19.0%) SS content

are given in Fig. 3 with the second derivatives of the same two spectra in Fig. 4. No obvious difference can be seen in the shape of the optical density spectra due to differences in soluble solids content of fruit (Fig. 3). Second derivative processing of optical density spectral data removes the baseline shifts (Hruschka, 1987) and produces spectra in which the differences between high and low SS fruit can be observed (Fig. 4). Second derivative processing also removes the offset in optical density spectra as shown in Fig. 1 due to variability in the intensity of radiation which penetrates to

Table 2. Regression parameters and statistics for calibrations.

Calibration ^z	R ^y	SEC ^x	WL ₁ ^w	WL ₂ ^v
BLC93	0.98	0.52	902	888
BLC94	0.91	0.48	902	884
BLC95	0.93	0.42	827	907
ENC93	0.98	0.38	885	952
ENC94	0.90	0.35	905	827
ENC95	0.86	0.59	907	890
RHC93	0.76	0.88	907	866
RHC94	0.80	0.66	901	950
RHC95	0.90	0.55	900	885
WBC93	0.79	1.22	902	882
WBC94	0.92	0.61	908	870
WBC95	0.96	0.51	904	883
BLC	0.95	0.73	886	902
ENC	0.92	0.79	890	882
RHC	0.97	0.37	885	906
WBC	0.96	0.63	883	904
PC93	0.95	0.72	905	886
PC94	0.95	0.53	902	890
PC95	0.96	0.76	886	900
PC	0.94	0.79	885	906

^zBL = 'Blake'; EN = 'Encore'; RH = 'Red Haven'; WB = 'Winblo'; C = a calibration data set; P = pooled (combined) data sets. The numerical designation indicates the production year (e.g., 93 = 1993). Therefore, BLC93 = 'Blake' calibration data set for 1993.

^yMultiple correlation coefficient.

^xStandard error of calibration.

^wFirst selected wavelength.

^vSecond selected wavelength

inner tissue, caused by nonuniform surface light scattering in peach fruit. The subtle effect due to soluble solids can then be seen as given in Fig. 4. These differences are the basis for the quantitative determination of SS in intact fruit. Figure 4 shows that the use of second derivative processing enhances the variation in spectral data especially in the 860 to 920 nm region. It also produces a smoothing effect that reduces spectral noise.

Calibration statistics and selected wavelengths for the multiple linear regression models are given in Table 2. The multiple correlation coefficients (*R*) of individual cultivar calibrations ranged from 0.76 for RHC93 to 0.98 for BLC93. The cultivar and season calibrations had higher *R* values above 0.93. The standard errors of calibration (SEC) for individual cultivar calibrations ranged from 0.35% to 1.22%. The cultivar and season calibrations had SEC values ranging from 0.37% for RHC to 0.79% for ENC and PC. Overall calibration (PC) had a *R* value of 0.94 with a SEC of 0.79%. The relationship between laboratory determined SS content to that calculated by the overall calibration PC is shown in Fig. 5.

Typically the two selected wavelengths in the calibration model fell between 870 to 910 nm indicating that the information related to the SS content of fruit was contained in this region of the NIR spectra. These wavelengths are very close to those reported by other researchers working on fruit and vegetable quality assessment using NIR techniques. Slaughter (1995) had selected optimum wavelengths at 910 nm and 872 nm in his regression model to predict SS in peaches and nectarines. Calibrations for determining onion SS content by Birth et al., (1985) used 878 to 897 nm and 900 to 908 nm in their regression models. NIR determination of SS in melons used wavelengths at 884 nm and 913 nm (Dull et al., 1992).

Bias, SEP and *r* of validation were used as criteria for evaluating the capability of a calibration model as a predictor of the SS level of independent samples. The fitness of the individual cultivar calibrations and season calibrations were evaluated by predicting the SS contents in the individual cultivar and season validation data sets in all possible combinations, separately for each season (Tables 3 to 5). Season calibrations and overall calibration were also tested by predicting SS contents of season and the overall validation (Table 6). Likewise, performance of cultivar calibrations and the overall calibration was evaluated by predicting SS levels in cultivar validations (Table 7).

Individual cultivar calibrations predicted SS contents in their respective individual cultivar validation data sets within the same season with comparatively little bias (−0.01% for BLC95 to 0.63% for ENC93). However, when one cultivar's calibration was used to predict SS content in another cultivar's validation within the same season, the bias was increased to as much as 2.64% when ENC93 predicted SS in RHV93 (Table 3). On the other hand, the season calibrations predicted individual cultivar validations within the same season with bias values ranging from 0.02% to 0.56% (Tables 3 to 5). When season calibrations were used to predict SS in season validations within the same season bias ranged from −0.01% to 0.29%. When season calibration was used to predict SS in season validations apart from the same season, bias ranged from as low as 0.01% to as high as −2.08%. Overall calibration predictions of SS levels in season and overall validation data sets by overall calibration PC yielded bias values ranging from 0.17% to −0.38% (Table 6). Cultivar calibrations predicted SS in respective cultivar validations with bias values ranging from −0.02% to −0.25% while predictions on other cultivar validations gave bias values that ranged from 0.05% to 1.62% (Table 7).

The highest SEP value observed for an individual cultivar calibration when used to predict its respective individual cultivar validation within the same season was 1.40% when ENC93 predicted SS levels in ENV93. ENC94 predicted its respective validation ENV94 with the lowest observed SEP of 0.49%. For the

Fig. 5. Relationship between laboratory determined peach soluble solids (SS) content to that calculated using the pooled calibration equation (PC).

Table 3. Bias, standard error of prediction (SEP) and simple correlation coefficient (r) of individual cultivar and season calibrations for 1993.

Validation ^z	Calibration				
	BLC93	ENC93	RHC93	WBC93	PC93
Bias (%)					
BLV93	-0.080	0.139	0.269	-0.545	0.232
ENV93	-0.229	0.625	-0.239	-0.891	0.558
RHV93	-1.170	2.640	0.221	-1.520	0.356
WBV93	-0.927	1.560	0.144	-0.532	0.015
PV93	-0.601	1.240	0.099	-0.873	0.292
SEP (%)					
BLV93	0.938	1.250	1.160	0.896	1.060
ENV93	1.520	1.400	1.630	1.560	1.500
RHV93	1.010	1.250	0.852	1.030	0.886
WBV93	1.380	1.530	1.330	1.340	1.360
PV93	1.260	1.590	1.330	1.260	1.270
r					
BLV93	0.806	0.615	0.683	0.824	0.745
ENV93	0.413	0.545	0.197	0.355	0.432
RHV93	0.644	0.328	0.763	0.620	0.741
WBV93	0.585	0.434	0.627	0.620	0.602
PV93	0.679	0.381	0.638	0.683	0.675

^zBL = 'Blake'; EN = 'Encore'; RH = 'Red Haven'; WB = 'Winblo'; V = a validation data set; C = a calibration data set; P = pooled (combined) data sets. The numerical designation indicates the production year (e.g., 93 = 1993). Therefore, BLC93 = 'Blake' calibration data set for 1993.

Table 4. Bias, standard error of prediction (SEP) and simple correlation coefficient (r) of individual cultivar and season calibrations for 1994.

Validation ^z	Calibration				
	BLC94	ENC94	RHC94	WBC94	PC94
Bias (%)					
BLV94	-0.20	0.72	-0.05	-0.45	-0.14
ENV94	-0.05	-0.05	-0.35	-1.53	0.06
RHV94	0.01	1.32	-0.24	-0.80	-0.18
WBV94	0.57	1.98	0.29	0.11	0.24
PV94	-0.01	0.11	0.99	-0.09	-0.67
SEP (%)					
BLV94	0.68	0.72	1.00	0.81	0.83
ENV94	0.55	0.49	0.70	0.53	0.61
RHV94	0.93	0.99	0.87	0.84	0.93
WBV94	0.87	0.89	1.24	0.86	1.05
PV94	0.90	1.32	1.01	1.00	0.97
r					
BLV94	0.84	0.82	0.62	0.77	0.76
ENV94	0.76	0.82	0.57	0.78	0.69
RHV94	0.41	0.20	0.51	0.57	0.40
WBV94	0.84	0.84	0.64	0.85	0.76
PV94	0.81	0.50	0.75	0.76	0.77

^zBL = 'Blake'; EN = 'Encore'; RH = 'Red Haven'; WB = 'Winblo'; V = a validation data set; C = a calibration data set; P = pooled (combined) data sets. The numerical designation indicates the production year (e.g., 94 = 1994). Therefore, BLC94 = 'Blake' calibration data set for 1994.

season calibrations the highest SEP of 1.50% was obtained when PC93 predicted SS in ENV93 while PC95 predicted SS in BLV95 with a SEP of 0.58% which was the lowest observed SEP for a season calibration predicting individual cultivar validations (Tables 3 to 5). Season calibration PC93 predicted SS in PV93 with a SEP

Table 5. Bias, standard error of prediction (SEP) and simple correlation coefficient (r) of individual cultivar and season calibrations for 1995.

Validation ^z	Calibration				
	BLC95	ENC95	RHC95	WBC95	PC95
Bias (%)					
BLV95	-0.01	1.23	-0.78	-1.30	-0.18
ENV95	-0.98	-0.02	-1.01	-2.12	-0.26
RHV95	0.89	1.35	-0.02	0.28	0.18
WBV95	1.58	2.06	0.18	-0.17	0.29
PV95	0.34	1.17	-0.40	-0.82	-0.01
SEP (%)					
BLV95	0.66	0.68	0.72	0.65	0.57
ENV95	1.02	0.94	1.12	1.07	1.03
RHV95	0.56	0.84	0.59	0.75	0.62
WBV95	0.95	1.00	1.10	0.94	1.16
PV95	1.16	1.11	1.15	1.24	0.90
r					
BLV95	0.59	0.55	0.49	0.61	0.72
ENV95	0.51	0.60	0.31	0.42	0.48
RHV95	0.90	0.77	0.89	0.82	0.88
WBV95	0.87	0.85	0.82	0.87	0.79
PV95	0.89	0.90	0.89	0.87	0.94

^zBL = 'Blake'; EN = 'Encore'; RH = 'Red Haven'; WB = 'Winblo'; V = a validation data set; C = a calibration data set; P = pooled (combined) data sets. The numerical designation indicates the production year (e.g., 95 = 1995). Therefore, BLC95 = 'Blake' calibration data set for 1995.

Table 6. Bias, standard error of prediction (SEP) and simple correlation coefficient (r) of season and overall calibrations.

Validation ^z	Calibration			
	PC93	PC94	PC95	PC
Bias (%)				
PV93	0.29	-2.08	-0.36	-0.20
PV94	0.93	-0.01	0.86	0.17
PV95	0.18	-1.98	-0.01	-0.38
PV	0.34	-1.63	0.01	-0.24
SEP (%)				
PV93	1.27	1.34	1.36	1.26
PV94	0.94	0.97	0.96	0.94
PV95	1.07	1.20	0.90	1.01
PV	1.16	1.41	1.18	1.11
r				
PV93	0.68	0.63	0.61	0.68
PV94	0.78	0.77	0.78	0.79
PV95	0.91	0.88	0.94	0.92
PV	0.83	0.74	0.82	0.85

^zP = pooled (combined) data sets; V = a validation data set; C = a calibration data set. The numerical designation indicates the production year (e.g., 93 = 1993).

value of 1.27% while that of PC95 was 0.90% when it predicted SS levels in PV95 (Table 6). The lowest SEP observed for a cultivar calibration was 0.93% when RHC predicted SS in RHV while ENC had the highest SEP of 1.55% when used to predict SS in WBV (Table 7).

The highest r value observed for an individual cultivar calibration was 0.89 for RHC95 while RHC94 had the lowest r value of 0.51 when those calibrations predicted their respective individual cultivar validations RHV95 and RHV94, respectively. Season calibration PC95 gave the highest r value of 0.88 when used to

Table 7. Bias, standard error of prediction (SEP) and simple correlation coefficient (r) of cultivar and overall calibrations.

Validation	Calibration				
	BLC	ENC	RHC	WBC	PC
	Bias (%)				
BLV	-0.25	0.07	-0.72	-0.60	-0.37
ENV	0.05	-0.08	-0.62	-0.54	-0.38
RHV	0.56	1.62	-0.02	0.75	0.12
WBV	0.33	0.61	-0.22	0.11	0.10
	SEP (%)				
BLV	1.01	1.19	0.95	0.95	0.92
ENV	1.24	1.13	1.28	1.32	1.37
RHV	0.99	1.14	0.93	1.07	0.92
WBV	1.35	1.55	1.14	1.20	1.14
	r				
BLV	0.83	0.75	0.85	0.85	0.86
ENV	0.76	0.81	0.74	0.73	0.70
RHV	0.71	0.59	0.75	0.66	0.76
WBV	0.81	0.73	0.87	0.85	0.87

^aBL = 'Blake'; EN = 'Encore'; RH = 'Red Haven'; WB = 'Winblo'; P = pooled (combined) data sets; V = a validation data set; C = a calibration data set.

predict SS in RHV95 while PC94 predicted SS in WBV94 with the lowest r of 0.40. The lowest r value in a cross validation was 0.20 when ENC94 predicted SS in RHV94 (Tables 3 to 5). Season calibrations and the overall calibration yielded r values ranging from 0.61 to 0.94 in cross validation of season and overall validation data sets (Table 6). The r values for cultivar calibrations in predicting cultivar validations were between 0.59 to 0.85 (Table 7).

Validation statistics indicate that individual cultivar calibrations are successful, i.e., predictions have lower bias, lower SEP and higher r values, while predicting SS in the same cultivar's validation data set within the same season. However, such calibrations were not successful in consistently predicting the SS content of other cultivars within the same season as shown by bias values as much as 2.64% higher in one instance (Table 3). On the other hand, season and cultivar calibrations as well as the overall calibration were successful in predicting the SS content of individual cultivar, season and cultivar validation data sets. The relationship between laboratory determined SS content of the overall validation data set (PV) to that predicted by using the overall calibration (PC) is shown in Fig. 6. Even though PV had 600 spectra, the validation results are reported only for 500 spectra which is the maximum capacity of NSAS program for a single validation.

It is important to note that even though individual cultivar calibrations had slightly lower R and low SEC values compared to combined calibrations, they were not good predictors most of the time when the cultivar was different. Many sample factors including chemical composition, interaction between chemical constituents, and moisture status of samples affect the performance of calibrations (Williams, 1987). Flinn and Murray (1992) demonstrated sample, instrumental, and seasonal influences on the performance of NIR calibrations in feed analysis. It is possible that differences in physical and chemical composition among cultivars may have caused the observed performance of individual cultivar calibrations. However, these results also indicate that the cultivar or season calibration can be successfully employed to predict the SS content of fruit from different cultivars in different seasons.

The success of a NIR calibration depends on the spread in sample composition relative to the error inherent in the chemical

reference method, the relative diversity of the calibration and validation sets, and whether it is robust enough to embrace all sources of variation in unknown samples when applied to open sample populations (Flinn and Murray, 1992). Different cultivars of fruit may have substantial differences in their chemical and physical properties (Ahmed and Denninson, 1971; Bourne, 1979; Robertson and Scorza, 1989). These differences in chemical and physical properties may lead to differences in optical properties, possibly due to variations in light scattering behavior of fruit skin and flesh. A more refined and robust calibration may be obtained with the incorporation of more cultivars to account for more sources of variation in physical and chemical characteristics in addition to SS content. This is important for instruments intended for fruit when the cultivar is not known. On the other hand our results suggest that if the cultivar is known, it is best to use a calibration derived for the particular cultivar.

A high gradient of SS content exists around and across peach fruit and as a consequence, measurement will vary with both the location and volume of tissue sampled for analysis. Our observations with SS levels measured on two halves of 40 fruit (10 fruit from each cultivar) demonstrated a maximum difference of 1.7% with a mean of 0.47% and a standard deviation of 0.43%. The SS content of fruit tissue ranged from 11.9% to 15.4% when tissue samples were taken from different locations on a medium size fruit. These observations point out that several readings should be taken from an individual fruit, regardless of the method of analysis, and averaged to get a representative value. This can be easily and quickly achieved using the NIR method described.

Our results confirm that a strong predictable relationship exists between NIR absorbance and SS content of peaches. It is possible

Fig. 6. Relationship between laboratory determined peach soluble solids (SS) content in the pooled validation (PV) data set and that predicted by pooled calibration (PC) data set.

that this technique could be employed in packing-line sorting of fresh market and processing peaches. It takes about 10 s to scan one fruit 10 times over the range of 800 to 1050 nm. However, scanning time can be significantly reduced by narrowing the range of spectra since only a narrow spectral band (≈ 865 to 920 nm) is needed. In addition, with the availability of more sensitive spectrometer components and fiber optics, fruit scan time should be substantially reduced. Using the technique described, fruit could be graded into two or three sweetness classes with a fairly high degree of precision. It should be possible, therefore, to develop portable instruments which will allow the measurement of SS at different stages in the production-marketing chain allowing growers, sellers, and buyers to rapidly and nondestructively assess fruit quality. At the same time, additional research is needed to assess the potential of measuring other critical fruit quality characteristics modulating consumer acceptance. Incorporation of this technology should be highly beneficial to the peach industry, improving the quality and consistency of the product marketed and in turn, improving consumer confidence in peach quality.

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