IMPROVEMENT OF NIR TRANSMISSION MODE FOR INTERNAL QUALITY ASSESSMENT OF FRUIT USING DIFFERENT ORIENTATIONS

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ABSTRACT

In the last decade, visible and near-infrared spectroscopy (including three modes reflectance, interactance and transmission) has increasingly been utilized in food industry. In this research, transmission mode was used to acquire spectra of kiwifruits, apples and oranges in the range of 400–1,000 nm, with an emphasis on the effect of fruit orientation on the spectra pattern. For soluble solids content and acidity (pH) to be predicted, various calibration models were developed, based on different combinations of preprocessing techniques. The best model for each characteristic was obtained by standard normal variate transformation in combination with median filter and first derivative. The correlation coefficients for soluble solids content and pH were 0.93 and 0.943, and the root mean square errors of prediction for them were 0.259°Brix and 0.076, respectively. The results indicate that the occurrence of peaks is uniquely the inherent of the fruit, independent of orientation. The transmission calibration model for the estimation of fruit constituents could be improved by using proper preprocessing techniques.

PRACTICAL APPLICATIONS

Near-infrared spectroscopy (NIRS) for food quality assessment has its own advantages in comparison with other nondestructive techniques. The

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accuracy of NIR models is usually more than the other techniques. It is fast, easy to use and noninvasive. Moreover, there is no need for reagents, and minimal or no sample preparation is required. Because of these advantages, NIRS has been used in many fields including grains, beverages, dairy product, processed food, fruits and vegetables for determination of water, proteins, fats, carbohydrates, starch, amino acid, ash, soluble solid content, pH and so on. NIRS have shown promise as a fast, nondestructive and low-running-cost technique. It is also a nondestructive tool for the determination of organic component concentration. NIRS can be applied in different areas of food industry. This wide range of NIRS applications demands more gradual research to make it more efficient and practical.

INTRODUCTION

Quality assurance and evaluation of food for fresh markets and processing industries have become an important and fundamental issue because of increased quality expectation of consumers. Final acceptance of products by consumers is strongly influenced by internal quality attributes. Besides, food safety and quality are directly related to people's health and social improvement (Cen and He 2007). However, quality evaluation of food, including fruits and vegetables, can be difficult because their complex composition complicates quantitative and qualitative determination of the individual constituents. Moreover, most of the quality measuring methods involve complex processing of samples and require some expensive chemical reagents with considerable amount of labor-intensive works. Furthermore, most of these methods are still destructive. Thus, it is essential to develop efficient and nondestructive methods for measuring internal attributes of fruits. In this regard, it has been shown that NIRS is a promising technique with fast, easy-to-use, nondestructive and analytical features (Day and Fearn 1982) that can be carried out online (Osborne *et al.* 1993; Hoyer 1997) or in-line (Singh Sahni *et al.* 2004). Minimum or no sample pretreatment is necessary, which places it among rapid techniques (Day and Fearn 1982; Osborne 2000). One of the main advantages of NIR spectroscopy is the simultaneous measurement of several constituents. Besides, the components as low as 0.1% concentration could be detected and evaluated by NIRS (Cen and He 2007).

These features of NIRS have encouraged the researchers to utilize this technique for quality assessment of different food such as rice (Lu *et al.* 2007), wheat (Cocchi *et al.* 2006), milk (Maraboli *et al.* 2002), meat (Geesink *et al.* 2003) bread (Xie *et al.* 2004), barely (Munck *et al.* 2004), apple (Yan-de *et al.* 2007), pear (Sirisomboon *et al.* 2007) and kiwifruit (McGlone *et al.* 2002).

Schaare and Fraser (2000) compared three modes of visible–near-infrared spectroscopic measurement (reflectance, interactance and transmission) for their ability to nondestructively estimate harvest soluble solids content (SSC), density and internal flesh color of the yellow-fleshed kiwifruit (*Actinidia chinensis*). They found that the spectra of interactance mode provided the most accurate estimates of SSC, density and flesh color. Consequently, McGlone *et al.* (2002) compared the interactance mode of NIRS with density method for prediction of dry matter and SSC of kiwifruits. They reported that the accuracy of the NIRS and density methods were fairly similar. They could predict SSC of kiwifruits with $R^2 = 0.92$ and the root mean square error of prediction (RMSEP) was 0.39%. Afterward, Clark *et al.* (2004) used the interactance mode with the same equipment and procedures of McGlone *et al.* (2002) in order to predict the storage disorders of kiwifruits (*A. chinensis*). Fu *et al.* (2007) compared the transmission and reflectance modes of visible (VIS) spectroscopy/NIRS using a very sensitive spectrometer for detecting brown heart in pears. With such a spectrometer, better results were obtained based on transmission spectra than those of reflectance spectra. The classifying correctness of transmission mode was 91.2%. However, each mode of spectroscopy has its pros and cons.

Although the interactance mode provides a more accurate estimation of kiwifruit attributes than reflectance and transmittance modes, obtaining a light seal may be difficult at the high conveyor speeds used in current fruit grading systems. Reflectance mode measurements are the easiest to obtain because they require no contact with the fruit. However, in this mode, the required light levels are relatively high. Moreover, variations in superficial or surface properties of the fruit may influence the calibrations (Schaare and Fraser 2000). Fu *et al.* (2007) reported that the reflectance spectra had only contained spectral information of the surface layer, whereas the light transmitted through the fruit contained not only the spectral information of the surface layer but also the information of inner flesh tissues. However, in transmission mode, the amount of light penetrating the fruit is very small, which results in a reduced signal-to-noise ratio for transmission spectra compared with those obtained for interactance and reflectance modes (Schaare and Fraser 2000). The authors expected that the transmission mode could provide better evaluation of fruit internal attributes than interactance and reflectance modes, if more intense light, suitable positioning of fruit and appropriate preprocessing techniques were employed.

The objective of this study was to improve the transmission mode calibrations for kiwifruit internal quality predictions using a more intense light, an ordinary spectrometer and different combinations of preprocessing techniques for effective noise removal. Several calibration models were developed for accurate prediction of SSC and acidity (pH) of kiwifruit. Furthermore, the transmission mode was used for kiwifruits along with apples and oranges in two different orientations in order to show that each fruit has its individual spectra independent of the spectra acquisition orientation, which can be used for quality evaluation. There have been few studies that directly investigate the effects of fruit orientations on the pattern of transmission spectra.

MATERIALS AND METHODS

Fruit Samples

Experiments were performed with 10 samples of each fruit for comparison purpose of the spectra. Moreover, in order to develop the calibration models and evaluate their validity, a total of 100 kiwifruits were randomly divided into two groups: the first one was for models' calibration (70 samples) and the other group of samples was for predictions of quality and model validation purposes (30 samples). Samples were individually numbered and stored for 2 days at 20°C and 60% relative humidity. After spectra acquisition, SSC was measured by using a digital refractometer (Schmidt + Haensch, Berlin, Germany). The acidity (pH) of samples was also measured by a pH meter (Hanna HI model: 8519, Padova, Italy). All experiments including spectra acquisition and quality analysis were carried out on the same day.

Spectra Measurement

Transmission spectra was measured in the range of 400–1,000 nm with 1-nm interval by using spectrometer (Jasco FP-6200, Tokyo, Japan) equipped with Spectra Manager software for Windows (Jasco, Tokyo, Japan) (Fig. 1).

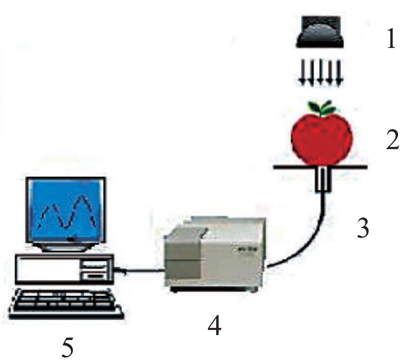

FIG. 1. VIS/NIRS EXPERIMENTAL INSTRUMENT SET UP FOR TRANSMISSION MODE (V): (1) LIGHT SOURCE; (2) SAMPLE; (3) FIBER OPTIC; (4) SPECTROMETER; AND (5) COMPUTER

Intact samples were placed on the fruit holder with two different orientations: stem-calyx axis vertical (T_V) and stem-calyx axis horizontal (T_H). The fruit holder was used with a flexible shield between the fruit sample and the fiber probe, which acted as a light seal against a light source. An Osram tungsten halogen lamp 300 W that could emit visible and infrared radiation was put above the sample and at a distance of 50 mm from the fruit surface. The transmitted light through samples was directed to the detector of spectrometer via an optic fiber. In a vertical orientation setup (T_V), the samples were irradiated by the light source from above, toward the stem and detected by the optic fiber from the calyx. While in a horizontal orientation setup (T_H), the samples were irradiated by the light source from a cheek and detected from the opposite cheek by the optic fiber.

Data Analysis and Modeling

The data acquired from NIR spectrometer contain sample information besides background information and unwanted noise. Hence, spectral preprocessing techniques are required to remove any irrelevant information, including noise, in order to obtain reliable, accurate and stable calibration models (Cen and He 2007). In this study, several preprocessing methods in conjunction with their different combinations were used. These were normalization (multiplicative scatter correction [MSC], standard normal variate transformation [SNV]), smoothing (median filter, Savitzky-Golay and wavelet) and differentiation (first [D^1] and second [D^2] derivative). All preprocessing techniques and calibration methods were carried out by means of ParLeS software version 3.1 (Viscarra Rossel 2008; University of Sydney, Australia). The effect and application of these preprocessing methods are briefly presented hereinafter:

Normalization. Normalization is designed to remove multiplicative spectral effects. In normalization, the spectral vector is transformed into unit length (Swierenga *et al.* 1999). SNV reduces multiplicative effects of scattering, particle size and multicolinearity changes over all the NIR spectra (Zeaiter *et al.* 2005). MSC is used to compensate for additive (baseline shift) and multiplicative (tilt) effects in the spectral data, which are induced by physical effects (Nicolaï *et al.* 2007).

Smoothing. Smoothing is a preprocessing method for noise reduction, represented by random changes in amplitude from point to point within the signal. Smoothing is therefore necessary in order to optimize the signal-to-noise ratio (Zeaiter *et al.* 2005). Median filter, as a spectra smoothing method, can be used for spike removal. It is very crucial to choose the proper Median filter rank, which was 4 in this study.

Differentiation. The roles of differentiation is to remove the background and to enhance spectral resolution. A constant background is removed by transforming the original spectra into first derivative spectra, and a linear background is eliminated by transforming them into the second derivative spectra (Condolfi *et al.* 1999).

Prior to modeling by partial least squares (PLS), the spectra variation was analyzed by using principal component analysis (PCA) to eliminate defective spectra outliers (Shao *et al.* 2007). Three samples for SSC and one sample for pH were left out from the calibration set because of their potential bad influences over the models. PLS method was then used to develop calibration models to predict SSC and pH of kiwifruits. PLS found the directions of greatest variability by considering both spectral and measured property information, with the new axes called PLS factors (Blanco and Villarroya 2002). The prediction error of the calibration model was defined for a different sample set as the RMSEP:

$$RMSEP = \sqrt{\frac{\sum_{i=1}^{n_p} (\hat{y}_i - y_i)^2}{n_p}}, \tag{1}$$

where $\hat{y}_i$ is the predicted value of the ith observation, y_i is the measured value of the ith observation and n_p is the number of observations in the prediction set.

RESULTS AND DISCUSSIONS

Comparison of Different Orientation

The spectra of some kiwifruit samples with T_H orientation (horizontal positioning) are shown in Fig. 2. From this figure, despite different percentage of transmitted light, all transmission spectra followed the same pattern. The amount of light transmitted depends on the fruit properties such as size, shape, defect, firmness and internal cavity. As a result, fruits have various percentage of transmitted light. The spectra of kiwifruits had two peaks almost at the same wavelength: approximately at 560 and 721 nm.

The average spectra of kiwifruit samples acquired with T_H and T_V orientations are shown in Figs. 3 and 4, respectively. It can be seen that, for T_V orientation also, the transmission spectra had two peaks with the same wave-

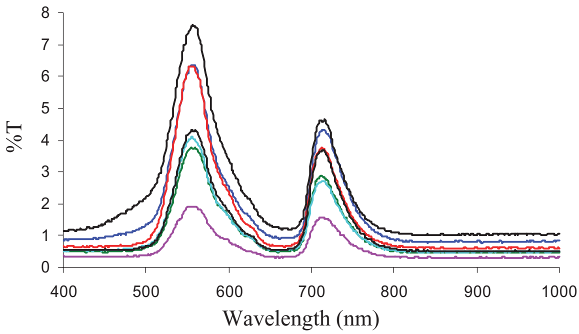

FIG. 2. ORIGINAL TRANSMISSION SPECTRA OF KIWIFRUITS (T_H)

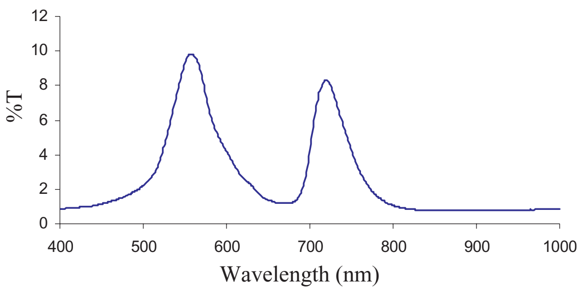

FIG. 3. AVERAGE TRANSMISSION SPECTRA OF KIWIFRUITS (T_H)

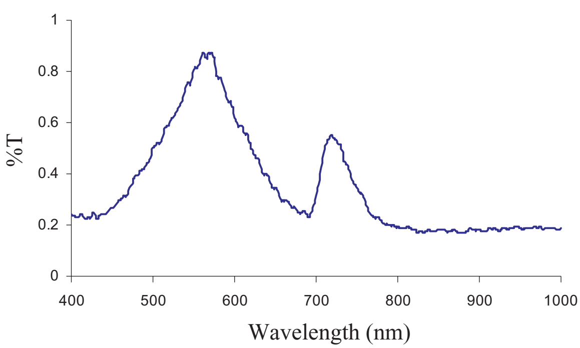

FIG. 4. AVERAGE TRANSMISSION SPECTRA OF KIWIFRUITS (T_V)

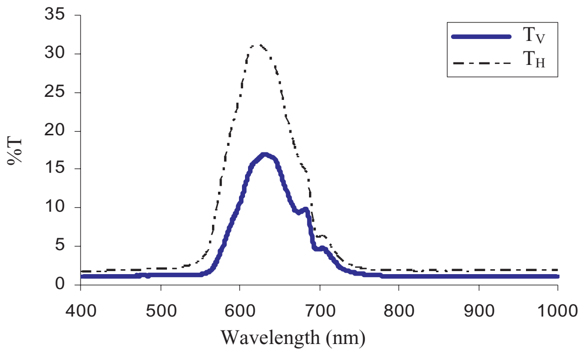

FIG. 5. AVERAGE TRANSMISSION SPECTRA OF ORANGES

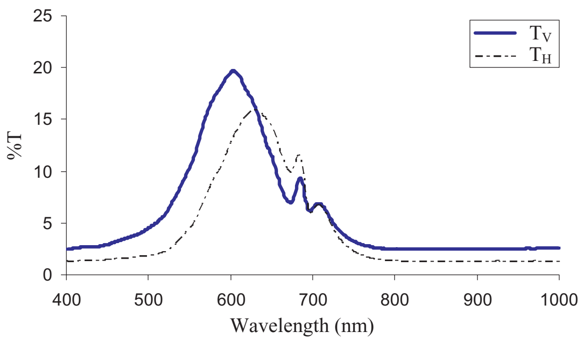

FIG. 6. AVERAGE TRANSMISSION SPECTRA OF APPLES

lengths of T_H orientation. This assures that the occurrence of transmission spectra peaks inherently depends upon the constituents of fruits. However, the percentage of transmitted light in T_V orientation was several times less than in the T_H orientation. This was mainly a result of the difference between the path lengths of traveled light through the fruit in two orientations and the difference between the tissue of kiwifruits in longitudinal and transverse directions. Consequently, the amount of light transmitted through the fruit in vertically positioned kiwifruits (T_V) was very small and therefore resulted in a reduced signal-to-noise ratio in comparison with its horizontal positioning (T_H).

The average spectra of oranges and apples are presented in Figs. 5 and 6, respectively. It is seen that, for each fruit, both orientations T_V (stem–calyx axis vertical) and T_H (stem–calyx axis horizontal) have the same pattern but with different percentage of transmitted light. The spectra of apples had three peaks, approximately at 631, 683 and 707 nm, whereas, for oranges, there were two peaks, at about 622 and 704 nm. It can be concluded that the occurrence of the peaks is uniquely the inherent of fruits independent of orientation and concentration of fruit constituents, while the percentage of transmitted light can be related to the properties of fruit.

The percentage of transmitted light of apples in T_H orientation was less than its T_V orientation. However, this difference was not considerable because apples could be considered as a spherical fruit, and the path length of light through apple in both orientations was roughly similar.

The amount of transmitted light for oranges in T_H orientation was more than its T_V orientation. This difference was higher than for apples but was not as much as for kiwifruits because the pith and peel firmness of the stem and calyx parts are more than the cheek area of oranges. Therefore, light could hardly penetrate through oranges from the stem or calyx.

Because kiwifruits are considered as an elliptical fruit, with a big difference between the percentage of transmitted light of its two orientations, the horizontal orientation was utilized for spectra acquisition and modeling step. Moreover, kiwifruits have higher price than apples and oranges in Iran. Thus, the prediction of its internal attributes is given priority over other fruits.

Development of Different Preprocessing for Calibration Models

Various calibration models were developed by using different preprocessing techniques on the spectral data. Each calibration model was used to predict SSC and pH of prediction data set in order to verify the superior ability of models based on different preprocessing techniques. A proper model should have low RMSEP and high correlation coefficient between the predicted and measured value of each property. Moreover, a low number of PLS factors is desirable in order to avoid inclusion of signal noise in the modeling (Xiaobo *et al.* 2007). The models have been developed by using different numbers of PLS factors and different combinations of preprocessing techniques. However, only the most proper models were presented in Tables 1 and 2 with their correlation coefficient and RMSEP. If no preprocessing is applied, a minimum correlation coefficient is observed in the 10-factor PLS model for the prediction of either SSC or pH. However, if preprocessing is applied, correlation coefficient increases and RMSEP is reduced. In the meantime, it was found that, by performing the preprocessing of data, the number of PLS factors is reduced. It can be seen that the best preprocessing is SNV in combination with median filter and first derivative. This combination increased the correlation coefficient from 0.6 to 0.93 and from 0.808 to 0.943 for prediction of SSC and pH, respectively. Meanwhile, RMSEP decreased from 0.551 to 0.259 for SSC and from 0.142 to 0.076 for pH, and the number of PLS factors dropped to 9.

As previously mentioned, each preprocessing is used for a specific purpose, and they yield to different results. SNV removes the multiplicative

TABLE 1.
THE RESULTS FOR PREDICTION OF SSC WITH DIFFERENT PREPROCESSING TECHNIQUES

Preprocessing	No. of PLS factor	*r*	RMSEP
Original data	10	0.60	0.551
SNV, Median filter, D^1	9	0.93	0.259
SNV, Savitzky-Golay, D^1	10	0.796	0.386
SNV, Wavelet, D^1	6	0.791	0.401
SNV, Median filter, D^2	8	0.657	0.765
SNV, Median filter, D^1 and mean center	8	0.92	0.262
SNV, Median filter, D^2 and mean center	5	0.905	0.271
MSC, Median filter, D^1	9	0.921	0.474
MSC, Savitzky-Golay, D^1	9	0.798	0.388
MSC, Wavelet, D^1	6	0.824	0.673
MSC, Median filter, D^2 and mean center	4	0.904	0.272

MSC, multiplicative scatter correction; PLS, partial least squares; RMSEP, root mean square error of prediction; SNV, standard normal variate; SSC, soluble solid content.

TABLE 2.
THE RESULTS FOR PREDICTION OF pH WITH DIFFERENT PREPROCESSING TECHNIQUES

Preprocessing	No. of PLS factor	*r*	RMSEP
Original data	10	0.808	0.142
SNV, Median filter, D^1	9	0.943	0.076
SNV, Savitzky-Golay, D^1	10	0.936	0.086
SNV, Wavelet, D^1	10	0.926	0.097
SNV, Median filter, D^2	8	0.791	0.162
SNV, Median filter, D^1 and mean center	8	0.934	0.08
SNV, Median filter, D^2 and mean center	7	0.928	0.088
MSC, Median filter, D^1	9	0.943	0.244
MSC, Savitzky-Golay, D^1	10	0.945	0.214
MSC, Wavelet, D^1	10	0.904	0.235
MSC, Median filter, D^2 and mean center	10	0.93	0.085

MSC, multiplicative scatter correction; PLS, partial least squares; RMSEP, root mean square error of prediction; SNV, standard normal variate.

interferences of scatter and particle size, whereas MSC removes additive baseline besides multiplicative signal effects. However, the advantage of SNV over MSC is that SNV is applied to an individual spectrum, whereas MSC uses a “reference spectrum”, such as the mean spectrum of the calibration set. First derivatives (D^1) are applied to remove additive baseline effects, and second derivatives (D^2) are used to remove sloped additive baselines (Swierenga *et al.* 1999). Cen and He (2007) concluded that first derivative exhibited better results than second derivative, as the peaks and volleys not very obviously in original spectra become clearer by first derivative. Median filter eliminates the spikes of the spectral. As a result of removing these identifiable spikes, the signal-to-noise ratio is improved, and the spectrum looks more reasonable. The results showed the effects of different preprocessing techniques on the prediction performance of the model using PCA and PLS methods.

Prediction of Internal Quality Characteristics

Having known the best preprocessing of the model, PLS prediction results for SSC (Fig. 7) and pH (Fig. 8) of kiwifruits are presented as scatter plots. In both figures, the ordinate and abscissa axes represent the predicted and measured fitted values of the appropriate parameters, respectively. The prediction performances of these models were excellent with high correlation coefficient and low RMSEP for each characteristic.

The best model for the prediction of SSC was developed when SNV, median filter and first derivative were used as preprocessing and a nine-factor PLS model was found to be sufficient for the prediction of the SSC of intact

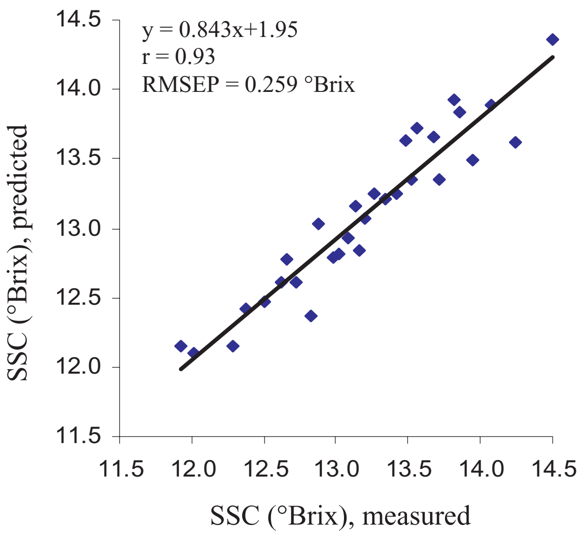

FIG. 7. SCATTER PLOTS OF MEASURED VERSUS PREDICTED SSC USING SNV, MEDIAN FILTER AND FIRST DERIVATIVE

RMSEP, root mean square error of prediction; SSC, soluble solid content; SNV, standard normal variate.

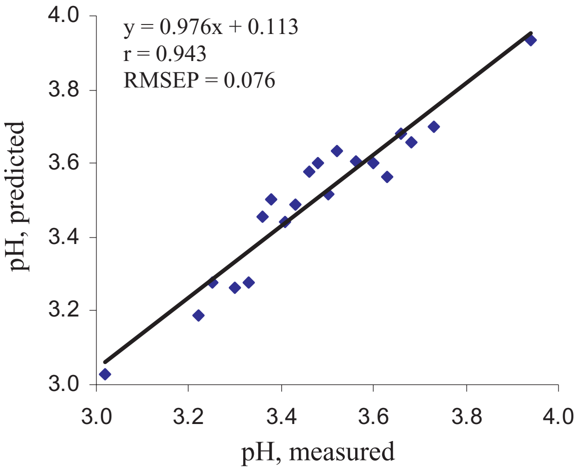

FIG. 8. SCATTER PLOTS OF MEASURED VERSUS PREDICTED PH USING SNV, MEDIAN FILTER AND FIRST DERIVATIVE

RMSEP, root mean square error of prediction; SNV, standard normal variate.

kiwifruits. The correlation coefficient between the measured and the predicted SSC for best model was as high as 0.93, with RMSEP 0.259°Brix (Fig. 7).

Any research is directly affected by its materials and methods (including sample, equipment for spectra acquisition, methods of spectra acquisition and developing calibration models). Hence, the outcome results may be different from others because of the variation in materials and methods. The values of regression coefficient of SSC obtained in this research are slightly superior to those obtained by Shao *et al.* (2007) in tomatoes with $r = 0.90$ and RMSEP = 0.377; by Lu (2001) in the cherries Sam variety with $r = 0.89$ and SEP = 0.65; by Peirs *et al.* (2001) with values between $r = 0.73$ and 0.89 in different apple varieties; by Lammertyn *et al.* (1998) in apples with $r = 0.82$ and SEP = 0.6; and by Slaughter *et al.* (1996) in tomatoes with $r = 0.89$ and SEP = 0.33. On the other hand, better results have been found in Satsuma mandarins with $r = 0.94$ and RMSEP = 0.325°Brix (Gomez *et al.* 2006), and in Cherries Hedelfinger variety with $r = 0.97$ and SEP = 0.71 (Lu 2001). However, the RMSEP achieved in this research (RMSEP = 0.259°Brix) was lower than those obtained by others (e.g., McGlone *et al.* [2002] with RMSEP = 0.39% and Clark *et al.* [2004] with RMSEP = 0.76% in kiwifruits).

The best model for prediction of pH was achieved when SNV, median filter and first derivative were used as preprocessing and a nine-factor PLS calibration model was appropriate for determining the pH of intact kiwifruits. The correlation coefficient between the measured and the predicted pH for the best model was as high as 0.943, with RMSEP 0.076 (Fig. 8).

The regression coefficients of pH obtained in this study was slightly superior to those obtained by Shao *et al.* (2007) in tomatoes with $r = 0.83$ and RMSEP = 0.251; by Gomez *et al.* (2006) in Satsuma mandarins with $r = 0.805$ and RMSEP = 0.179; and by Lammertyn *et al.* (1998) in apples with $r = 0.93$ and SEP = 0.068.

CONCLUSIONS

In recent years, NIRS has been utilized to evaluate the quantity and quality of food, including fruit, vegetables, beverage, processed food and dairy products. NIR with transmission mode is suitable for internal quality assessment of fruits, as it passes through the fruit flesh and, hence, has the spectral information of fruit internal properties besides the surface layer of fruits. However, the percentage of light penetrating the fruits is usually very low and resulted in a reduced signal-to-noise ratio because water, which is the main constituent of most fruits and vegetables, highly absorbs near-infrared radiation.

The transmission spectra of apples, oranges and kiwifruits were acquired with two different orientations: stem–calyx axis vertical (T_V) and stem–calyx axis horizontal (T_H). The results showed that the spectrum obtained from specific fruit follows a similar pattern that is independent of fruit orientation. However, the amount of transmitted light and, hence, the signal to noise ratio, may change with orientation, particularly for elliptical fruit such as kiwifruits. For this reason, when employing NIRS with transmission mode, it is recommended to find and choose a suitable orientation with higher percentage of transmitted light to obtain a better signal-to-noise ratio. For elliptical fruits such as kiwifruits, this usually occurs with horizontal orientation.

In this study, the transmission mode was utilized for kiwifruit internal quality prediction. Despite employing ordinary equipments, we could achieve reliable and accurate results when appropriate preprocessing techniques besides more intense light were used. Different combinations of preprocessing techniques were applied to remove any irrelevant information including noise and background information. The best model for nondestructive prediction of SSC and pH were developed when SNV, median filter and first derivative were performed as preprocessing. The correlation coefficients to SSC and pH were 0.93 and 0.943, and RMSEP for them were 0.259°Brix and 0.076, respectively. It can therefore be concluded that transmittance mode of NIR can successfully predict the internal quality of fruits if a suitable preprocessing technique is employed. More efforts can be performed to assess the feasibility of transmittance mode for internal quality prediction of fruit with a bigger size where the percentage of transmitted light is very crucial.

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