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Prediction of Soluble Solids Content of Chestnut using VIS/NIR Spectroscopy

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Abstract

Purpose: The present study focused on the estimation of soluble solids content (SSC) of chestnut using reflectance and transmittance spectra in range of VIS/NIR. **Methods:** Four species intact/peeled chestnuts were used for acquisition of spectral data. Transmittance and reflectance spectra were used to develop the best PLS model to estimate SSC of chestnut. **Results:** The model developed with the transmitted energy spectra of peeled chestnuts rather than intact chestnuts and with range of NIR rather than VIS performed better. The best R^2 and RMSEP of cross validation were represented as 0.54 and 1.85 °Brix. The results presented that the reflectance spectra of peeled chestnuts by species showed the best performance to predict SSC of chestnut. R^2 and RMSEP were 0.55 and 1.67 °Brix. **Conclusions:** All developed models showed RMSEP around 1.44 ~ 2.54 °Brix, which is considered not enough to estimate SSC accurately. It was noted that R^2 of cross validation that we found were not high. For all that, grading of the fruits in two or three classes of SSC during postharvest handling seems possible with an inexpensive spectrophotometer. Furthermore, the development of estimation of SSC by each chestnut species could be considered in that SSC distribution is clustering in different range by species.

Keywords: Cross validation, Chestnut, NIR spectroscopy, PLS, Prediction of SSC

Introduction

Chestnut (Castanea spp.) is popular for its abundant nutrients and delicious taste in Asia and Europe (Liu et al., 2011). More than 2,000,000 ton chestnuts were produced annually, and the consumption and production of chestnut continue to rise all over the world according to the Food and Agriculture Organization statistics (FAO, 2011). In particular, Korea is a large chestnut consumer and the biggest chestnut importer and exporter. Considering the rate of processed food such as roast chestnut, dried chestnut and chestnut flour increases rapidly owing to consistent researches and developments of food processing techniques, it is noted that the research of grading and non-invasive measurement of the internal quality is requested in order to improve the amount of export of high-quality chestnuts (Chen and Sun, 1991).

Visible and Near-infrared (NIR) spectroscopy in combination with some chemometrics regression approaches to process monitoring and fault detection has become an established method for rapid and nondestructive assessment of quality parameters in the food and agricultural sectors (Donis-Gonzalez et al., 2012). NIR spectroscopy was first used in agricultural applications by Norris and Hart (1965) to measure moisture in grain. Since then it has been used for rapid analysis of mainly moisture, protein and fat contents of a wide variety of agricultural and food products (Gunasekaran, 2001; Suh et al., 2012). Early applications in horticulture focused on dry matter

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content of onions (Birth et al., 1985), soluble solids content (SSC) of apples (Zude et al., 2006) and water content of mushrooms (Roy et al., 1993), but since then many other applications have followed. Recent developed system which extended the potential of NIR spectroscopy further includes multi- and hyperspectral imaging techniques which also provided spatial information (ElMasry et al, 2008) and time-resolved spectroscopy which allowed the measurement of absorption and scattering processes separately (Cubeddu et al., 2001). The on-line non-contact spectroscopic measurements are the only measuring techniques that can meet these demands, and the NIR spectroscopy has proven to be an extremely reliable and informative spectral technique.

Generally, chestnut quality is measured not only by external factors such as color, shape, size, surface status and surface mold growth, but also by internal qualities which are important for consumer acceptance. Most importantly, the external appearance usually is not altered, at least initially, by sugar content making them difficult to determine without destructive evaluation. Besides, measurement of the chestnut quality is sorted and classified according to SSC related with sugar content and nutrition components using traditional chemical methods. However, the traditional methods are time-consuming, laborious and expensive. Thus, the study was to investigate the non-invasive method of chestnut quality with reliable detection technology. Also, the primary aim for the study was to ascertain whether SSC of intact and peeled chestnuts could be estimated by VIS/NIR spectroscopy or not.

Materials and Methods

Chestnut preparation

Chestnut samples used for spectra acquisition in range of VIS/NIR were four species. Samjoseng and Okwang were obtained from on-line market and harvested at Kong-ju, the southern area of Korea in October 2010. Daebo and Enki species harvested at Suwon in 2010 were supported from the Korea Forest Research Institute, and stored at cold storage around 0℃ for 2 months. All samples were exposed to temperature 24℃ over 2 h before experimental tests to allow for temperature equilibrium. The basic properties of chestnuts used in experiments are shown in Table 1.

Overall procedure for performing the experiment was set like Figure 1. The prepared chestnuts after tempering over 2 h were measured the basic properties such as weight and volume. Volume measurement was completed using Equation 1, and then the spectra were measured before and after peeing outer hull. Continuously, 1 mm slices with the half of peeled chestnut were dried to measure the moisture content (MC) in the dry oven (C-DHD2, Chang shin scientific co., Korea) at 105℃ for 6 h. The other half was squeezed and used for SSC measurement by a digital refractometer (PR-101, ATAGO, Japan).

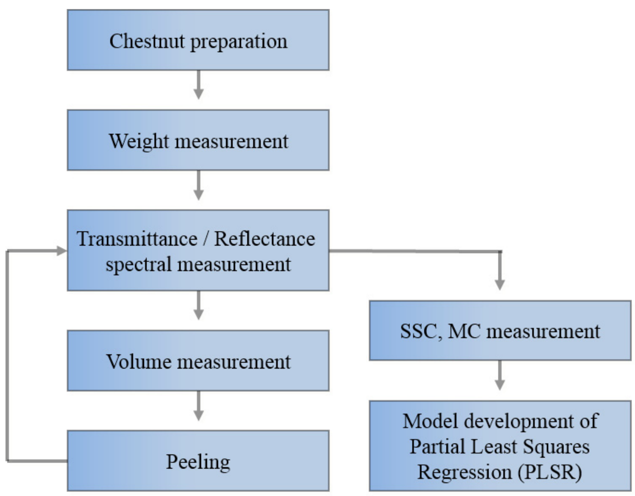

Figure 1. The procedure of measurement and spectra acquisition of chestnuts.

Table 1. Basic property of chestnut samples (mean ± standard deviation)

Species	Number of samples	Weight (g)	Density (g/cm^2)	MC (%)	SSC (˚Brix)
Samjoseng	183	25.74±3.69	1.09±0.07	63.92±3.85	16.61±2.48
Okwang	135	20.94±2.34	1.07±0.02	62.33±2.82	25.47±1.89
Daebo	230	20.15±1.99	1.07±0.02	65.75±4.35	22.85±2.95
Enki	140	23.50±2.68	1.04±0.02	64.68±3.22	20.11±2.76
Total	688	21.87±3.83	1.07±0.04	64.37±3.69	21.14±4.14

$$V = \frac{W_a - W_w}{\gamma_w} = \frac{W_{bfw} - W_{bw}}{\gamma_w} = \frac{W_d}{\gamma_w} \quad (1)$$

where,
W_a = Weight an of object in the air
W_w = Weight of an object in the water
W_{bfw} = Total weight of (object + container + water)
W_{bw} = Weight of (container + water) in the air
W_d = Buoyancy of an object

Spectral acquisition

Three different spectrophotometers were used to obtain transmitted energy and reflectance spectra of intact and peeled chestnuts as shown in Table 2. The spectra acquisition was implemented as shown in Figure 2. ColoMate spectrometer was not used for transmittance spectra measurement because it is incongruent for the setup of transmittance spectra acquisition. Three 1000 w Halogen lamps used as a light source were installed in a dark room for transmitted energy spectra, and the integrating sphere was composed for reflectance spectra. Circular area of 10 mm in diameter on a flat surface of intact/peeled chestnut samples was used for the reflectance spectra acquisition.

Table 2. Specifications of spectrometers

Item	Descriptions by spectrometer		
Manufacturer Model	SCINCO ColorMate	Ocean Optics USB2000	Control Development Inst. CDI NIR-128L
Wavelength range	270-1000 nm	520 -1186 nm	904 -1700 nm
Wavelength interval	5nm	10 nm	12.5nm
Light source	Pulsed Xenon lamp	Tungsten-halogen	Tungsten-halogen

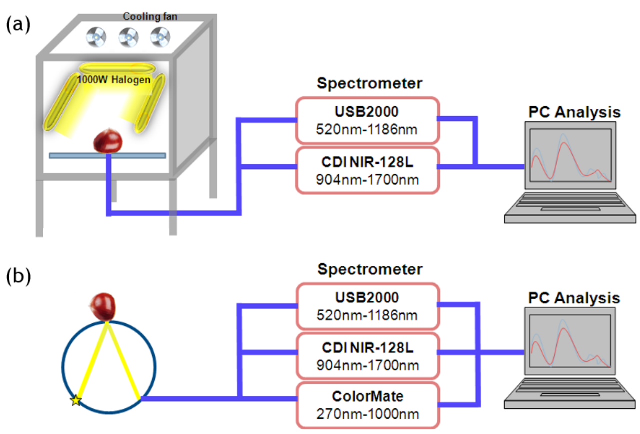

Figure 2. Features of transmitted energy spectra (a) and reflectance spectra (b) acquisition.

Statistical analysis

Partial least square regression (PLSR) model was developed using a commercial software (Unscrumbler 9.7, CAMO Software AS, Norway). The spectral data were conducted with moving average and multiplicative scatter correction (MSC) in order to investigate the best pre-treatment. The pre-treatment was also performed with the software.

The estimation model of SSC in chestnuts with spectral data was developed using a PLS regression with full cross validation. The PLS model has been described in detail in several researches (Khodabux et al., 2007). In order to avoid over-fitting of the model, the optimum number of terms in the PLS calibration model was determined as indicated by the lowest number of factors that gave the closest to minimum value of the prediction residual error sum of squares (PRESS) function in cross validation. The performance capacity was represented as values such as determination coefficient (R^2) and root mean square error of prediction (RMSEP).

Results and Discussion

Estimation of SSC in chestnut with VIS/NIR spectroscopy

Entire transmitted energy spectra by species of intact/peeled chestnuts with two spectrometers were as shown in Figure 3. Based on the features of spectra, all chestnuts had relatively lower transmittance energy intensity, and there is no clear difference among species. Comparing the spectra of lower SSC group and higher SSC group, it seemed difficult to distinguish the SSC of samples because of the overlapping and similarity of the spectra in entire region. A big difference between the intact and peeled in visible range exists, but it indicated that the graphs were similar in NIR region. Therefore it was determined that the PLS model development should be tried with VIS and NIR region separately.

PLS analysis results were shown in Table 2. RMSEP of the model with the intact chestnut was about 1.85 to 2.11 °Brix, and that of the peeled was about 1.95 to 2.25 °Brix. Developed models with NIR spectra performed better than with VIS spectra. However, it showed RMSEP around 1.85 ~ 2.25 °Brix, which means not enough to

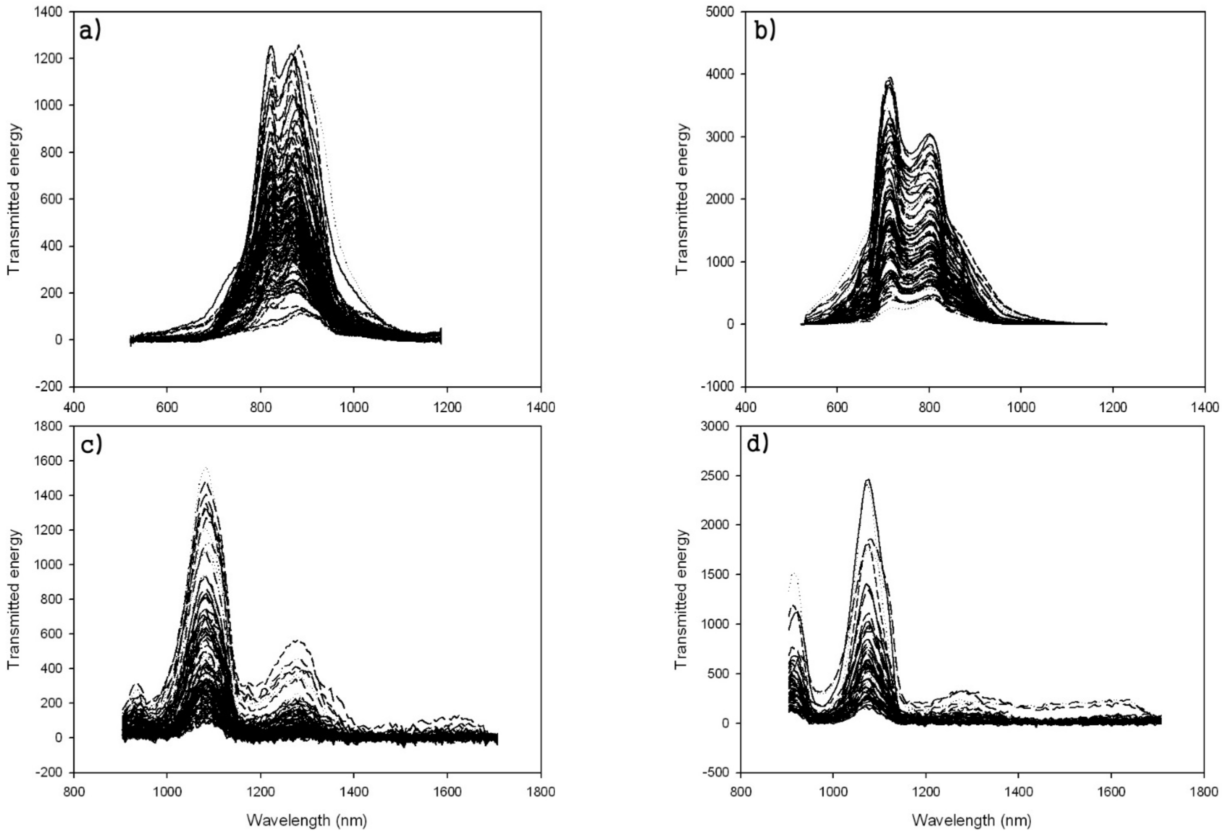

Figure 3. The NIR spectra of all species; a) Intact chestnuts with USB2000, b) Peeled chestnuts with USB2000, c) Intact chestnuts with CDI NIR-128L, d) Peeled chestnuts with CDI NIR-128L.

Table 3. The results for calibration and validation models of PLS methods for transmitted energy spectra of Daebo and Samjoseng species

Sample and used spectrometer (Wavelength range)	Pre-processor	Intact		Peeled	
		R_C^2	RMSEC	R_C^2	RMSEC
		R_V^2	RMSEP	R_V^2	RMSEP
Deabo USB2000 (520 nm-1,186 nm)	O	0.30	1.95	0.42	1.68
		0.21	2.11	0.25	1.95
	X	0.60	1.47	0.29	2.02
		0.31	1.95	0.16	2.25
Samjoseng CDI (904 nm-1,700 nm)	O	0.67	1.54	0.65	1.68
		0.51	1.90	0.48	2.07
	X	**0.70**	**1.50**	0.65	1.68
		0.54	**1.85**	0.50	2.01

estimate SSC accurately. The calibration and validation results of the optimum model based on the lowest RMSEP with the transmitted energy spectra were shown in Figure 4.

Based on the obtained reflectance spectra with USB2000, ColorMate and CDI NIR-128L, a big difference exists between the spectra before and after peeling, but no difference between chestnut species. The average spectra of peeled and intact chestnuts with ColorMate and USB2000 are shown in Figure 5. All reflectance spectra were used to develop the PLS model to estimate SSC in chestnuts.

Considering on the performance results shown in Table 4, the best performance on validation with developed

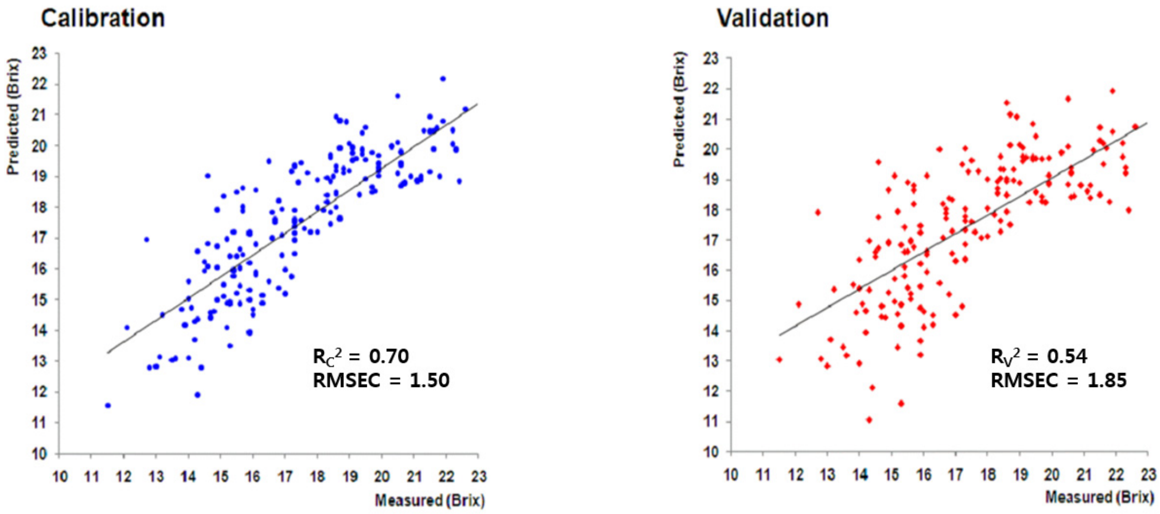

Figure 4. Predicted and measured values of SSC for the prediction set using a PLS model with the transmitted energy spectra of the intact Samjoseng samples.

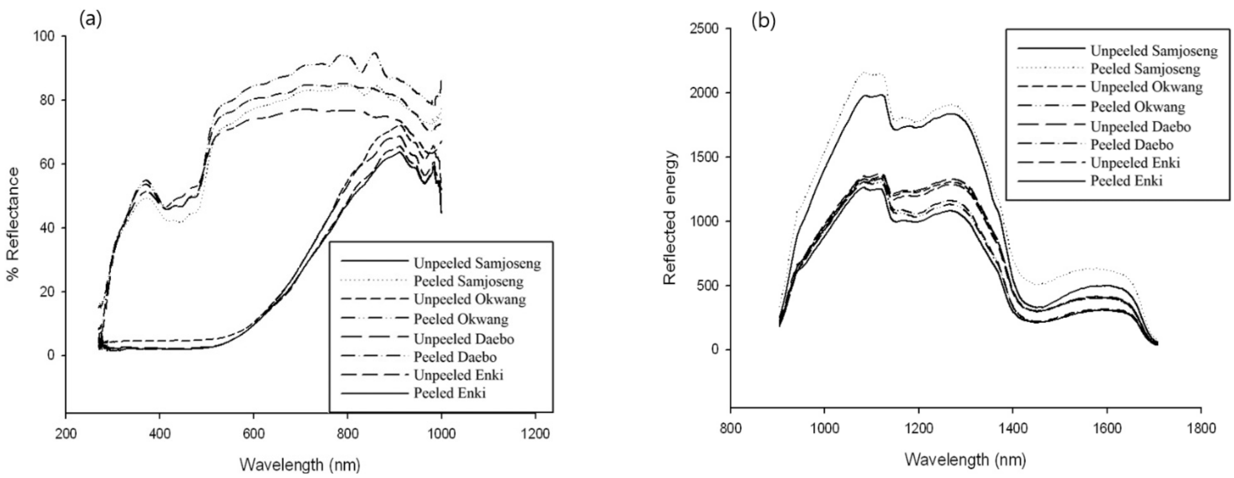

Figure 5. The average spectra of peeled and intact chestnuts; Percent reflectance spectra with ColorMate, b) Reflected energy spectra with USB2000.

models was indicated when the model was developed with spectra in rage of NIR in the peeled chestnut. The reason why it showed as similar as the result with models using the transmitted spectra is related with the principle of NIR spectroscopy. It has been successfully used in the quantitative and qualitative analysis of farm products such as fruits. Because the NIR region related to vibration and combination overtones of the fundamental O-H, C-H, and N-H bonds, which are the primary functional groups of sugar.

The NIR reflectance spectroscopy has been used to determine the physical and chemical properties and concentrations of various products (Wang, 2010). The best results with reflectance spectra of each species showed in range of NIR and the spectra of peeled samples were more significant than those of intact samples, and then obtained reflectance spectra with CDI NIR-128L spectrometer showed that R_C^2, R_V^2 and RMSEP values were 0.65, 0.52 and 1.702 °Brix, respectively.

Generally, the results of spectral analysis showed R_V^2 under 0.65 and RMSEP values over 1.5. It is determined that the developed model by each species was not suitable to predict SSC precisely. However, the classifications to two or three levels of SSC could be considerable to be determined.

The more PLS model was developed with the reflectance spectra of all peeled species additionally and the results are shown in Table 5. The best performance of PLS model showed that R_C^2, R_V^2 and RMSEP were 0.73, 0.72 and 2.18 °

Table 4. The results for calibration and validation of PLS model with reflectance spectra by chestnut species

Species	Samjoseng				Okwang				Daebo				Enki			
Spectrometer	Intact		Peeled		Intact		Peeled		Intact		Peeled		Intact		Peeled	
	R_C^2	RSC	R_C^2	RSC	R_C^2	RSC	R_C^2	RSC	R_C^2	RSC	R_C^2	RSC	R_C^2	RSC	R_C^2	RSC
	R_V^2	RSP	R_V^2	RSP	R_V^2	RSP	R_V^2	RSP	R_V^2	RSP	R_V^2	RSP	R_V^2	RSP	R_V^2	RSP
ColorMate	0.68	1.40	0.72	1.31	0.13	1.76	0.15	1.74	0.47	2.46	0.65	1.67	0.34	2.23	0.63	1.68
	0.61	1.54	0.55	1.67	0.04	1.86	0.07	1.83	0.40	2.63	0.47	2.08	0.14	2.56	0.50	1.96
CDI-NIR	0.65	1.461	0.75	1.25	0.21	1.67	0.25	1.63	0.60	1.79	0.50	1.91	0.33	2.25	0.45	2.04
	0.52	1.702	0.66	1.44	0.15	1.75	0.16	1.74	0.21	2.26	0.41	2.11	0.16	2.55	0.40	2.14

* RSC=RMSEC, RSP=RMSEP

Table 5. The results for calibration and validation of PLS model with reflectance spectra of entire species

Used spectrometer	Entire species			
	Intact		Peeled	
	R_C^2	RMSEC	R_C^2	RMSEC
	R_V^2	RMSEP	R_V^2	RMSEP
USB2000	0.59	2.02	0.55	2.08
	0.39	2.45	0.46	2.29
ColorMate	0.68	2.36	0.71	2.24
	0.65	2.47	0.66	2.40
CDI-NIR	0.67	2.39	0.73	2.16
	0.62	2.54	0.72	2.18

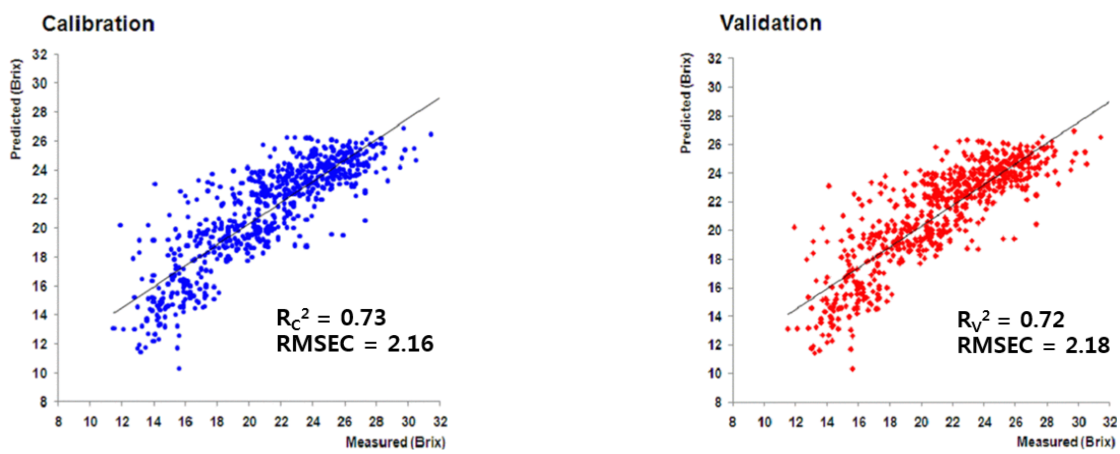

Figure 6. Predicted and measured values of SSC for the prediction set using a PLS model with the reflectance spectra of the all peeled species.

Brix, respectively. Figure 6 illustrates the calibration and validation scatter plot of the PLS model with the NIR reflectance spectra of the all peeled species. All models indicated determination of coefficients lower than 0.8. Regarding SSC distributions with clustering were different by each species, the development of estimation model for SSC by each species would be more reasonable.

Conclusions

In this study, it was verified that VIS/NIR spectroscopy is a feasible tool for quantification of inner qualities such as SSC in chestnuts with reasonable prediction errors over the entire content ranges measured. Four species intact/peeled chestnuts were used to develop the estimation model for SSC using reflectance and transmitted energy spectra in range of VIS/NIR. PLS models developed with spectra in range of VIS/NIR of intact and peeled chestnuts indicated similar performance capacity. All developed models showed RMSEP around 1.44 ~ 2.54 °Brix, which is considered not enough to estimate SSC accurately. It must be noted that the coefficients of determination (R^2) that we found were not high. Nevertheless, grading of the fruits in two or three classes of SSC during postharvest handling seems possible with an inexpensive spectrophotometer such as what we used. It must be decided whether to extend the calibration to more species or compute a different calibration for each species analyzed.

Conflict of Interest

No potential conflict of interest relevant to this article was reported.

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