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Measurement of soluble solids content in watermelon by Vis/NIR diffuse transmittance technique*

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Abstract: Watermelon is a popular fruit in the world with soluble solids content (SSC) being one of the major characteristics used for assessing its quality. This study was aimed at obtaining a method for nondestructive SSC detection of watermelons by means of visible/near infrared (Vis/NIR) diffuse transmittance technique. Vis/NIR transmittance spectra of intact watermelons were acquired using a low-cost commercially available spectrometer operating over the range 350~1000 nm. Spectra data were analyzed by two multivariate calibration techniques: partial least squares (PLS) and principal component regression (PCR) methods. Two experiments were designed for two varieties of watermelons [Qilin (QL), Zaochunhongyu (ZC)], which have different skin thickness range and shape dimensions. The influences of different data preprocessing and spectra treatments were also investigated. Performance of different models was assessed in terms of root mean square errors of calibration (RMSEC), root mean square errors of prediction (RMSEP) and correlation coefficient (r) between the predicted and measured parameter values. Results showed that spectra data preprocessing influenced the performance of the calibration models. The first derivative spectra showed the best results with high correlation coefficient of determination [r=0.918 (QL); r=0.954 (ZC)], low RMSEP [0.65 °Brix (QL); 0.58 °Brix (ZC)], low RMSEC [0.48 °Brix (QL); 0.34 °Brix (ZC)] and small difference between the RMSEP and the RMSEC by PLS method. The nondestructive Vis/NIR measurements provided good estimates of SSC index of watermelon, and the predicted values were highly correlated with destructively measured values for SSC. The models based on smoothing spectra (Savitzky-Golay filter smoothing method) did not enhance the performance of calibration models obviously. The results indicated the feasibility of Vis/NIR diffuse transmittance spectral analysis for predicting watermelon SSC in a nondestructive way.

Key words: Diffuse transmittance, Visible/near infrared, Nondestructive detection, Soluble solids content, Watermelon
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INTRODUCTION

Determination of fruit and vegetable quality is very important for both producers and processors. Watermelon as a delicious fruit has been widely accepted in the world and its internal quality is important for consumers and merchants. The current favorite way for checking a watermelon is to sense sound or vibration by slapping or rapping it. It is time consuming, tedious, and subject to error. Several studies on assessing the quality of watermelon based on its acoustic or vibration properties (Yamamoto *et al*., 1981; Chen *et al*., 1996; Diezma-Iglesias *et al*., 2004; Nourain *et al*., 2005) have been reported but this method is likely to be influenced by the environment noise and vibration. Measurement of the optical properties of fruits and vegetables has been one of the most successful nondestructive techniques for assessing its quality property, such as sugar content, titratable acidity, vitamin content, and so on. From the later 1980s, near-infrared spectroscopy has gained wide acceptance in quality assessment of agricultural products and its applications include quantitative determinations of onions (Birth *et al*., 1985), potatoes (Dull *et al*., 1989a), cantaloupe (Dull *et al*.,

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1989b), melons (Dull *et al*., 1992), mandarin (Kawano *et al*., 1993), peach (Peiris *et al*., 1997), apple (Liu *et al*., 2005) and mangoes (Mahayothee *et al*., 2004). Soluble solids content (SSC), because of its importance for fruit quality evaluation, is mostly studied in a wide range of fruits, e.g., intact peaches (Slaughter, 1995), apples (Lammertyn *et al*., 1998; Peiris *et al*., 1999; Liu and Ying, 2004), pears (Chen and Shaw, 1999), sweet cherries (Lu, 2001) and prune (Slaughter *et al*., 2003). However, there is little reported about visible/near infrared (Vis/NIR) method used for determining the interior quality of intact watermelon.

SSC is one of the major characteristics used for assessing watermelon quality. This study aimed to obtain a rapid method for nondestructive SSC detection of watermelon by means of Vis/NIR diffuse transmittance technique.

The objectives of this study were (1) to examine the possibility using Vis/NIR diffuse transmittance method for measuring the SSC in intact watermelon, and to establish relationships between the nondestructive Vis/NIR transmittance spectra measurements and SSC of watermelon; (2) to investigate the influence of different spectra processing methods and different modelling methods on the prediction performance.

MATERIALS AND METHODS

Materials

Two experiments were designed: experiment 1: 50 “Qilin (QL)” watermelons were purchased from the local fruit market and stored for 2 d at 22~24 °C and 55% relative humidity in Sept. 2005; experiment 2: 103 “Zaochunhongyu (ZC)” watermelons were also purchased from the local fruit market and stored in the same environment condition as QL watermelon in Jan. 2006. In the first experiment, 36 watermelons were used for calibration and the others were used for prediction. And in the second experiment, 73 watermelons were used for calibration and the others were used for prediction. All samples were cleaned and numbered first. And then the maximum diameter, maximum height and weight of each watermelon were measured and recorded.

Diffuse transmittance measurement

Vis/NIR transmittance spectra of intact watermelons were acquired using a low-cost commercially available spectrometer operating over the range 350~1000 nm. The spectrometer was equipped with a grating (600 lines blazed at 500 nm), a detector, and an optical fiber (Vis/NIR wavelength range) to provide diffuse transmittance measurements. The light source was installed in a special arc lamp-chimney. Besides, the system (Fig.1) contains a fruit holder attached with flexible shield on the top. This flexible shield acted as both a light seal against light source and as a flexible support to accommodate watermelons with different shapes.

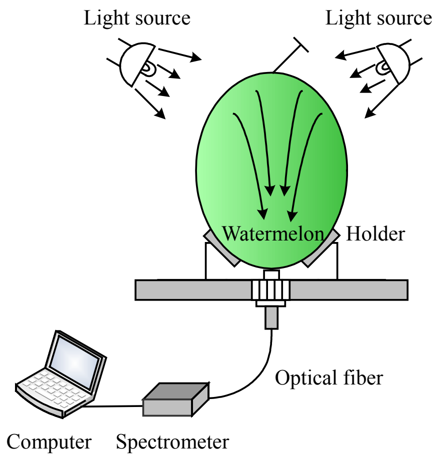


Fig.1 Schematic of spectra detecting system

Spectrometer parameters setting, spectra data collection and storing were carried out via a PC running specially developed software of the spectrometer. Samples were analyzed at room temperature (approximately 22~24 °C) without any previous sample treatment. The spectral curve was expressed as percent transmission (%T). The schematic of determination system and the determination flowchart are shown in Fig.1. Before fruit spectra acquisition, the background reference spectrum must be acquired by measuring the light source without being blocked by samples.

Samples were placed centrally and steadily upon the fruit holder during collection of transmittance spectra of intact watermelons with three methods

(Fig.2): stem-calyx axis 90° to horizontal (p1) (testing calyx position), calyx-stem axis nearly 90° to horizontal (p2) (testing stem position) which should guarantee stem not to affect NIR transmittance spectra collection and stem-calyx axis horizontal (p3) (testing equator position). Light from light source entered the fruit and diffused through the watermelon flesh. Then, the exiting light from the watermelon were received by detector and directed into the spectrometer through optics fiber. Three diffuse transmittance spectra were averaged to provide a mean spectrum for each watermelon.

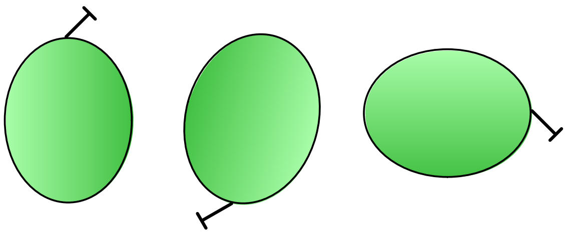


Fig.2 Methods of the watermelon on the fruit holder

SSC measurement

SSC (°Brix) of these watermelons were measured by a hand-held refractometer (Atago Co., PR-1 Brix-Meter, Tokyo, Japan). The juice that exuded from the total watermelon flesh was used as a sample. The value of SSC of each sample was obtained by averaging three determinations of the sample. Then the skin thickness was measured and recorded.

Data analyzing and modelling

Selection of the spectral wave band to be used in calibration is crucial and determines the quality of the model. Fig.3 shows the spectra of a QL sample and a ZC sample. From the figure, the two varieties of watermelons have similar transmittance spectra, and the wave crests of each spectrum were almost at the same wavelengths. As the detector is insensitive below 650 nm and becomes noisy above 950 nm, wavelengths from 650 nm to 950 nm were used for modelling in this study.

The commercial software package, TQ Analyst v6.2.1.509 Release, was used for data processing and

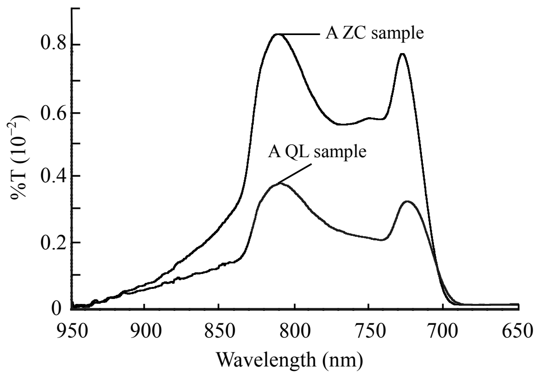


Fig.3 Original transmission spectra of a QL watermelon sample and a ZC watermelon sample

models development. Several pretreatment options and combinations were investigated including the first derivative of original spectra [D^1 (%T)], the second derivative of original spectra [D^2 (%T)], and spectra smoothing (Savitzky-Golay filter smoothing method). Once these preprocessing procedures were completed, partial least squares (PLS) and principal component regression (PCR) were used to develop calibration models for predicting the SSC.

In this study, the calibration model quality was quantified by the root mean square errors of calibration (RMSEC), the root mean square errors of prediction (RMSEP) and the correlation coefficient (r) between the predicted and measured parameter value. A good model should have a low RMSEC, a low RMSEP and a high r value, but also a small difference between RMSEC and RMSEP. The RMSEC and RMSEP are calculated as follows:

$$RMSEC=\sqrt{\frac{1}{I_{\mathrm{c}}-1}\sum_{i=1}^{I_{\mathrm{c}}}(\hat{y}_i-y_i)^2},$$

$$RMSEP=\sqrt{\frac{1}{I_{\mathrm{p}}-1}\sum_{i=1}^{I_{\mathrm{p}}}(\hat{y}_i-y_i-bias)^2},$$

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

$$bias=\frac{1}{I_{\mathrm{p}}}\sum_{i=1}^{I_{\mathrm{p}}}(\hat{y}_i-y_i).$$

RESULTS AND DISCUSSION

Samples

Table 1 shows the morphological properties of watermelon samples. The skin thickness of QL watermelons varied from 5 mm to 10 mm, and ZC watermelons varied from 3 mm to 7 mm. Any interpretation of calibration results depends greatly on the precision of the determined chemical composition of the samples. Table 2 summarizes the distributional statistics for SSC of calibration and prediction dataset.

Table 1 Morphological properties of watermelons used in the experiments

Watermelon	Parameter	Min	Max	Mean	*SD*
QL	Diameter (mm)	125.0	168.1	147.1	10.4
	Height (mm)	122.3	170.5	146.5	12.3
	Weight (g)	1004.5	2614.5	1647.1	371.0
ZC	Diameter (mm)	84.4	121.1	97.3	6.7
	Height (mm)	86.5	135.1	117.4	9.7
	Weight (g)	346.5	800.5	578.1	101.2

Table 2 Statistic values of calibration and prediction sets for SSC (°Brix)

Samples indexes	QL		ZC	
	Calibrations	Prediction	Calibrations	Prediction
N	36	14	73	30
Mean	9.11	9.01	9.90	9.96
Max	11.20	10.51	11.79	11.70
Min	6.60	7.40	7.01	8.01
SD	1.11	0.90	1.13	0.95

Statistical calibration models

It is desirable that a model has low calibration error, with as few factors as possible. The selection of calibration models based on this criterion was conducted by means of the TQ v6.2.1.509. The results for the calibration models of PLS and PCR for the original spectra %T, its first derivative D^1 (%T), and its second derivative D^2 (%T), are presented in Table 3.

It is obvious that the PLS method seems to produce the best calibration results using D^1 (%T) for SSC. PLS calibration results for SSC are presented in scatter plots, shown in Fig.4a (QL watermelons) and Fig.4b (ZC watermelons), respectively. The correlation coefficients (*r*) between the measured and predicted values of SSC are 0.918 (QL) and 0.954 (ZC), respectively. But PCR models produce a poor RMSEC.

Table 3 Results of PLS and PCR calibration models of %T, D^1 (%T), and D^2 (%T) in the wavelength range of 650~950 nm

Watermelon	Regression method	Statistical parameter	Spectrum (%T)		
			1	D^1	D^2
QL	PLS	No. of factors	7	6	3
		r	0.750	0.918	0.902
		RMSEC (°Brix)	0.76	0.48	0.49
	PCR	No. of PC	7	8	5
		r	0.568	0.700	0.467
		RMSEC (°Brix)	0.93	0.81	0.91
ZC	PLS	No. of factors	6	8	3
		r	0.812	0.954	0.843
		RMSEC (°Brix)	0.67	0.34	0.60
	PCR	No. of PC	6	4	6
		r	0.534	0.568	0.462
		RMSEC (°Brix)	0.96	0.92	0.99

Statistical prediction analysis

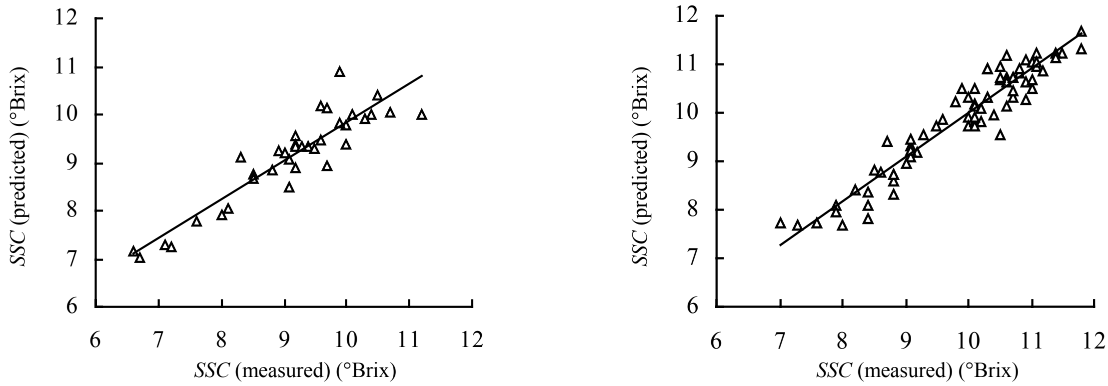
RMSEP represents the sensitivity of prediction. The results of these predictions are presented in Table 4.

Table 4 Results of PLS and PCR prediction models of %T, D^1 (%T) and D^2 (%T) for SSC in the wavelength range of 650~950 nm

Watermelon	Regression method	Statistical parameter	Spectrum (%T)		
			1	D^1	D^2
QL	PLS	No. of factors	7	6	3
		r	0.750	0.918	0.902
		RMSEP (°Brix)	0.97	0.65	0.84
	PCR	No. of PC	7	8	5
		r	0.568	0.700	0.467
		RMSEP (°Brix)	0.68	0.78	1.14
ZC	PLS	No. of factors	6	8	3
		r	0.812	0.954	0.843
		RMSEP (°Brix)	0.71	0.58	0.92
	PCR	No. of PC	6	4	6
		r	0.534	0.568	0.462
		RMSEP (°Brix)	0.84	0.94	0.90

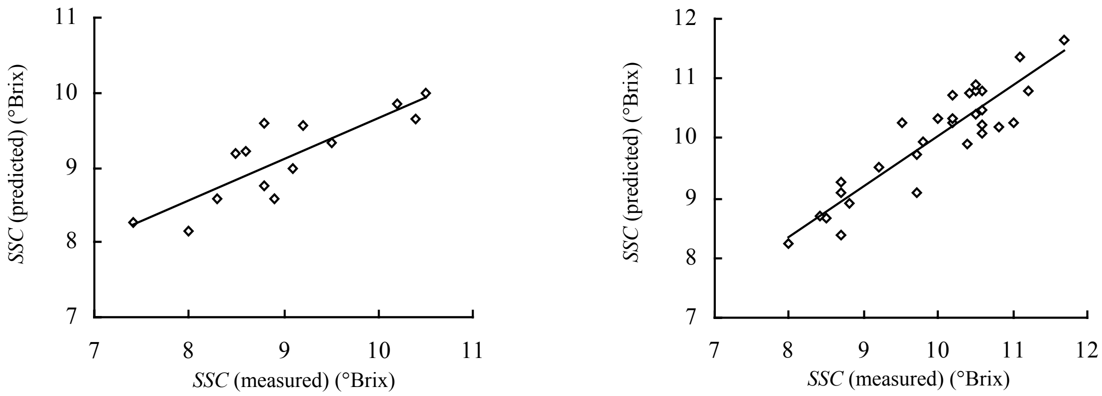
Comparison between PLS and PCR prediction results indicates that the PLS method is preferable. PLS prediction results for SSC are presented in scatter plots, in Fig.5a (QL) and Fig.5b (ZC) respectively. The correlation coefficients (*r*) between the measured and predicted values of SSC are 0.843 (QL) and 0.911 (ZC), respectively.

To evaluate the influence of spectra smoothing on calibration and prediction results, the Savitzky-Golay filter smoothing method was used in this research. The results for SSC calibration models of PLS and PCR methods for the original spectra %T, its first derivative D^1 (%T), and its second derivative D^2 (%T) using the smoothing method were investigated. Results showed that the spectral smoothing did not enhance the results of calibration models obviously. Some results for SSC calibration models of PLS regression method for first derivative D^1 (%T) are presented in Table 5.



(a) (b)

Fig.4 Scatter plots of measured versus predicted (a) QL and (b) ZC SSC for calibration model



(a) (b)

Fig.5 Scatter plots of measured versus predicted (a) QL and (b) ZC SSC for prediction model

Table 5 Results of PLS calibration models of D^1 (%T) using Savitzky-Golay filter smoothing method in the wavelength range of 650~950 nm

Watermelon	Data point	Polynomial order	Factors	*r*	*RMSEC*	*RMSEP*
QL	/	/	6	0.918	0.48	0.65
	7	4	7	0.883	0.51	0.66
	9	4	8	0.859	0.56	0.76
	11	4	7	0.836	0.60	0.78
ZC	/	/	8	0.954	0.34	0.58
	7	4	8	0.942	0.38	0.58
	9	4	7	0.883	0.53	0.53
	11	4	7	0.865	0.56	0.51

CONCLUSION

This research indicated that it is possible to develop a nondestructive technique for measuring watermelon SSC by Vis/NIR spectroscopy. Two experiments were designed for two varieties of watermelons which have different skin thickness range and shape dimensions, respectively. Multivariate calibration techniques (PLS and PCR) were used for establishing models of relation between diffuse transmittance spectra and SSC parameter of watermelon. Spectra data preprocessing influence the performance of the calibration models. The first derivative spectra showed the best results with high correlation coefficient of determination [r=0.918 (QL), r=0.954 (ZC)], low RMSEP [0.65 (QL), 0.58 (ZC)], low RMSEC [0.48 (QL), 0.34 (ZC)] and small difference between the RMSEP and the RMSEC by PLS method. The nondestructive Vis/NIR measurements provided good estimates of SSC index of watermelon, and the predicted values were highly correlated with destructively measured values for SSC. The models based on smoothing spectra did not enhance the results of calibration models obviously. The Vis/NIR diffuse transmittance technique will be valuable for nondestructive detecting of large shape, thick skin and not uniform component distribution fruits.

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