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Nondestructive Measurement of Soluble Solids Content in Pineapple Fruit Using Short Wavelength Near Infrared (SW-NIR) Spectroscopy

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Abstract

A nondestructive measurement of soluble solids content in pineapple fruit using short wavelength near infrared (SW-NIR) spectroscopy is proposed. The optimum conditions of measurement were investigated for spectra acquisition at an integration time of 150 ms and number of scanning of 100 scans. A number of 42 pineapple fruits were used as sample. The samples were divided into two groups, 24 samples for developing calibration model and 18 samples for performing validation test. The result showed that the best calibration model using short wavelength of 700-960 nm was identified with coefficient of determination (R^2) of 0.94 and standard error of prediction (SEP) of 0.88 % Brix. The calibration model resulted in high RPD value of 2.20.

Keywords: pineapple, SW-NIR, nondestructive measurement, soluble solids content

Introduction

The quality of pineapple fruit is measured not only by external factors such as color, shape and size but also by internal factors such as soluble solids content (SSC) and acidity. The SSC is considered to be the most important factor in determining the quality of pineapple fruit. The SSC is usually measured by using a refractometer but it is time-consuming, destructive and not free waste.

In the recent years, the use of near infrared (NIR) spectroscopy method both in the long wavelength and short wavelength for nondestructive quality evaluation of some fruits has been reported. In the long wavelength (1100-2500 nm), the use of this method for fruit quality evaluation is limited due to high moisture content of fruit (Krivoshiev, et al., 2000). In the short wavelength (700-1100 nm), the NIR spectroscopy method successfully determined the quality parameters of some fruits such as dry matter (DM), soluble solids content (SSC) and sugar content, nondestructively.

NIR spectroscopy successfully measured the DM of some fruits such as avocadoes (Clark et al., 2003), mango (Saranwong et al., 2003; Suhandy et al., 2007a) and kiwi fruit (McGlone and Kawano, 1998). NIR spectroscopy also successfully determined the SSC of some fruits such as apple (Lammertyn et al., 1998; Park et al., 2003), melon (Dull et al., 1992), mango (Suhandy et al., 2007b) and tomato (Slaughter et al., 1996; Khuriyati and Matsuoka, 2004). The sugar contents of apple (Lu et al., 2000), and orange (Kawano et al., 1993; McGlone et al., 2003) are also successfully measured by NIR spectroscopy method.

In this research, the potentiality of SW-NIR spectroscopy to measure the SSC of pineapple fruit was nondestructively evaluated. The correlation between the near infrared spectra in the short wavelength (700-1100 nm) and the SSC of pineapple fruit will be investigated. Then, a calibration model for nondestructive SSC determination in pineapple fruit using SW-NIR spectroscopy will be developed.

Materials and Method

Materials

A number of 42 pineapple fruits were hand harvested at the same time from the same orchard and used as samples. To get a broad range of SSC values, the samples consisting of three stages of maturation (i.e. 50% mature, 75% mature and 100% mature) were used. Then, the samples were divided into two groups, calibration and validation set. Table 1 shows the sample characteristics of pineapple used in this research.

Table 1: Statistical characteristics of sample used for developing calibration and validation model for SSC determination.

Items	Calibration Set	Validation Set
Number of sample	24	18
Range	11.25 – 18.44	11.87 – 17.89
Mean	14.76	14.74
Standard Deviation	1.85	1.94
Units	%Brix	%Brix

Method of spectral acquisition

Spectral acquisitions for each sample were taken at six different positions using the NIR spectrometer (VIS-NIR USB4000; Ocean Optics, USA). The spectra were stored in a computer for further analysis through the fiber optics. Since temperature affects fruit spectrum, the fruit temperature was maintained at 25°C by placing the sample into a water bath for 30 minutes. The measuring condition for spectral acquisitions was 150 ms for integration time and 100 scans for number of scanning. A ceramic plate (diffuse reflectance standard model WS-1, Ocean Optics, USA) was used as a reference. The intensity of light transmitted through the ceramic plate was measured, and then NIR measurement was performed by using a fruit in place of the ceramic plate. Spectral acquisition of the ceramic plate was made every time prior to the spectral acquisition of the fruit.

The absorbance spectra in the range of 300 nm to 1100 nm with 3 nm intervals for each fruit were measured. Spectra in the short near infrared region (700 nm to 1100 nm) were used for spectral analysis. The absorbance spectra was obtained by using the following formula:

$$A_\lambda = -\log_{10}\left(\frac{S_\lambda - D_\lambda}{R_\lambda - D_\lambda}\right) \quad (1)$$

where, S_λ = Intensity of sample at wavelength λ nm
D_λ = Intensity of dark at wavelength λ nm
R_λ = Intensity of reference at wavelength λ nm

Method of Soluble Solids Content (SSC) Measurement

The SSC of pineapple fruit was measured using refraktometer (Model IPR 201, Atago, Japan). For this purpose, a portion of pineapple flesh was cut at the point of spectral acquisition.

Data analysis

The average spectra from six positions were processed using smoothing (number of segments: 5) and Savitzky-Golay second derivative (left and right averaging: 33 nm, polynomial order: 2). Partial Least Squares (PLS) regression was used to develop a calibration model. All of these analyses were performed using The Unscrambler® version 7.01 (CAMO, Oslo, Norway), statistical software for multivariate calibration. A student's t-test was performed using Statistical Package for the Social Science (SPSS) version 11.0 for Windows in order to evaluate the significance level of the model.

Results and Discussion

Analysis of pineapple fruit spectra

The pineapple fruit spectra were measured in absorbance mode at six different positions. Then the original spectra for each sample were transformed to its smoothing and second derivative spectra. Fig. 1 depicts the second derivative of pineapple fruit spectra in SW-NIR region with high (16.11 Brix), middle (13.48 Brix) and low (11.99 Brix) SSC values. As shown in Fig. 1, different spectra were identified due to different SSC values.

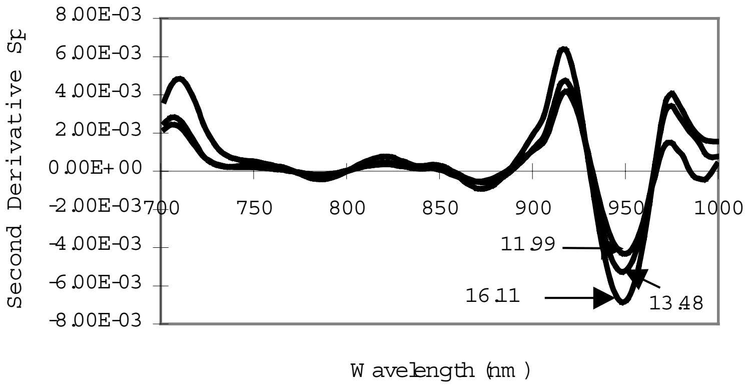

Figure 1: Second derivative of pineapple fruit spectra in the short near infrared wavelength with high, middle and low SSC values.

Developing a Calibration Model

Using the PLS regression method the calibration and validation was performed for original, smoothing and second derivative spectra (Table 2). Calibration model using the PLS method should have enough number of latent variable (LV) to optimize the prediction model and to avoid over-fitting. Furthermore, the best calibration model can be characterized as follows. These are low number of latent variable (LV), high coefficient of determination (R^2), low standard error of calibration (SEC), low standard error of prediction (SEP) and low bias. The ratio of standard error of prediction to standard deviation (RPD) value was the other parameter used for evaluating the performance of calibration model. For good prediction model, it is clearly understood that high RPD value is required (Williams, 1987).

Calibration model of original spectra at all wavelengths range resulted in high coefficient of determination (R^2 = 0.89–0.97). However, the calibration model for original spectra resulted in high standard error of prediction (SEP = 1.02–1.50). The number of latent variable for original spectra was high for all wavelength range (LV = 6–10). For this reason it should be considered as a case of over-fitting. In the second derivative spectra the number of latent variable was too high (LV = 14–15) and too low (LV = 1). High coefficient of determination was identified at some wavelengths range (R^2 = 0.96–0.98). However, those wavelengths range at the same time have a very high SEP values (SEP = 1.33–1.57). It is also a case of over-fitting.

In the smoothing spectra, the coefficient of determination was high (R^2 = 0.75–0.94). At the same time the SEP values were relatively low (SEP = 0.88–1.43). Then, the best calibration model was identified at wavelength range of 700–960 nm for smoothing spectra with R^2 = 0.94 and SEC = 0.47. This wavelength range has relatively low factor (F = 10) and low standard error of prediction (SEP = 0.88). For this wavelength range the ratio of standard error of prediction to standard deviation (RPD) value is also relatively high (RPD = 2.20).

Table 2: Calibration and validation results for SSC of pineapple fruit

Type of Spectra	**Wavelength (nm)**	**Latent Variable**	$\mathbf{R^2}$	**SEC**	**SEP**	**Difference between SEC and SEP**	**Bias**	**RPD**
Original Spectra	700-950	7	0.90	0.58	1.03	0.45	0.51	1.88
	700-960	6	0.89	0.62	1.03	0.41	0.46	1.89
	700-970	7	0.93	0.49	1.02	0.53	0.21	1.90
	700-980	9	0.96	0.37	1.10	0.73	0.35	1.76
	700-990	10	0.97	0.33	1.04	0.71	0.38	1.86
	700-1000	9	0.94	0.45	1.50	1.05	0.43	1.30
2nd Derivative Spectra	700-950	15	0.98	0.28	1.55	1.27	0.06	1.25
	700-960	1	0.22	1.63	1.78	0.15	-0.02	1.09
	700-970	14	0.96	0.36	1.48	1.12	-0.02	1.31
	700-980	15	0.97	0.32	1.33	1.01	-0.29	1.46
	700-990	14	0.97	0.31	1.57	1.26	0.02	1.23
	700-1000	1	0.22	1.64	1.80	0.16	-0.01	1.08
Smoothing Spectra	700-950	10	0.93	0.49	0.93	0.44	0.51	2.07
	700-960	10	0.94	0.47	0.88	0.41	0.40	2.20
	700-970	7	0.93	0.49	1.07	0.58	0.38	1.81
	700-980	9	0.94	0.43	1.29	0.86	0.32	1.5
	700-990	6	0.75	0.92	1.36	0.44	0.73	1.43
	700-1000	6	0.75	0.92	1.43	0.51	0.64	1.36

In order to clarify the behavior of the calibration model, the regression coefficient was plotted against the wavelength (Fig. 2). The wavelength of 756 nm contributed to build the calibration model. This wavelength corresponds with the absorbance band due to water (H_2O) in the second overtone (Osborne et al., 1993). The wavelength of 870 nm and 888 nm correspond with the absorbance band due to carbohydrate in several form such as starch, sucrose, fructose and glucose. These are the main component of SSC in fruit (Ho dan Hewitt, 1986). Khuriyati and Matsuoka (2004) used the wavelength of 884 nm for SSC prediction in tomato. Saranwong et al. (2003) used the wavelength of 878 nm to determine the SSC of mango.

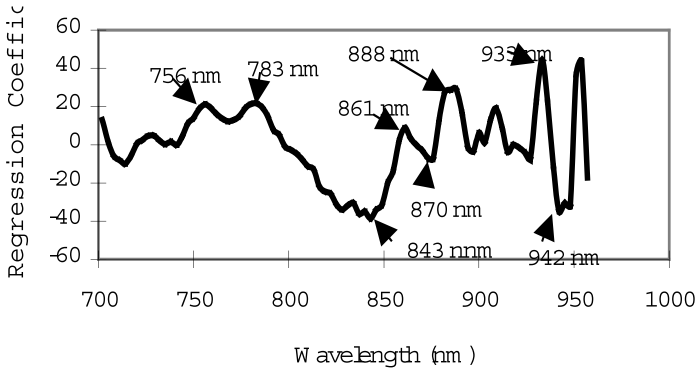

Figure 2: Regression coefficient plot for SSC calibration in wavelength range of 700-960nm.

Validation of Calibration Model

The validation of calibration model resulted in low SEP and low bias. Scatter plot between actual and predicted values is depicted in Fig. 3. By a 95% confidence pair *t-test*, there were no significant differences between the SSC of pineapple fruit measured using refraktometer and that predicted by near infrared spectroscopy. This result showed that a calibration model for nondestructive determination of SSC in pineapple fruit using short wavelength near infrared (SW-NIR) spectroscopy could be developed.

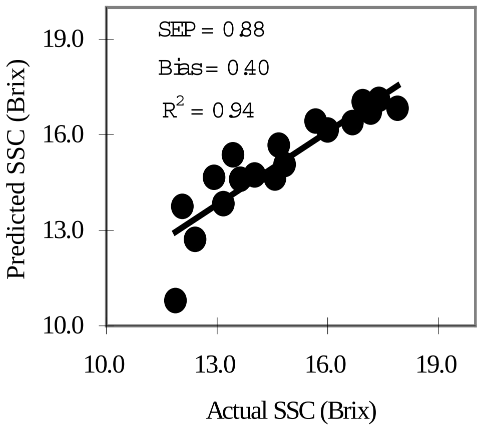

Figure 3: Scatter plot between actual and predicted SSC of pineapple fruit.

Conclusion

The nondestructive soluble solids content (SSC) measurement in pineapple fruit using SW-NIR spectroscopy was successfully proposed. The best calibration model was identified in the wavelength range of 700–960 nm for smoothing spectra with R^2 = 0.94 and SEC = 0.47. By a 95% confidence pair *t-test*, there were no significant differences between the SSC of pineapple fruit measured using refraktometer and that predicted by near infrared spectroscopy. This result showed that a calibration model for nondestructive determination of SSC in pineapple fruit using SW-NIR spectroscopy could be developed.

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