APPLICATION OF VISIBLE AND NEAR INFRARED SPECTROSCOPY FOR NONDESTRUCTIVE ANALYSIS OF TOMATO QUALITY

(Penerapan Visible dan Near Infrared Spectroscopy untuk Analisis Kualitas Tomat Secara Tidak Merusak)

Suparlan1) and Kazuhiko ITOH2)

1) Indonesian Center for Agricultural Engineering Research and Development (ICAERD), Situgadung, Tromol Pos 2 Serpong, Tangerang, Banten, 15310, Indonesia.
2) Graduate School of Agricultural Science, Hokkaido University, Kita 9, Nishi 9, Kita-ku, Sapporo 060-8589, Japan.

ABSTRACT

Near infrared spectroscopy has been used as a rapid and nondestructive method for determining the quality of fruit and vegetable. Calibration models of Visible Near Infrared (Vis-NIR) spectroscopy for color and soluble solids content (SSC) of fresh intact tomatoes was developed by partial least squares (PLS) regression analysis with a full cross validation method using 150 samples. The calibration model of color was developed using the wavelength ranged from 600 to 730 nm, and that of SSC was developed using the wavelength ranged from 700 to 1098 nm. Correlation coefficient of calibration (Rc2) and standard error of calibration (SEC) for color were 0.97 and 0.15, respectively, and those for SSC were 0.96 and 0.42 oBrix, respectively. The models were then used to predict color and SSC of an independent data set consist of 104 samples. The correlation coefficient of prediction (Rp2), the standard error of prediction (SEP), and the bias for prediction of color were 0.92, 0.19, and 0.09, respectively, and those for prediction of SSC were 0.91, 0.49 oBrix, and -0.04 oBrix, respectively. It was concluded that Vis-NIR spectroscopy interfaced with fiber optic is suitable method to determine color and SSC of fresh intact tomatoes. Thus, Vis-NIR technology could be used for classifying fresh intact tomatoes into qualitative groups based on both external and internal quality.

Keywords: nondestructive analysis; near-infrared spectroscopy; partial least squares regression; tomatoes quality;

ABSTRAK

Near infrared spectroscopy telah digunakan sebagai metode yang cepat dan tidak merusak dalam penentuan kualitas buah dan sayuran. Model-model kalibrasi dari "Visible Near Infrared (Vis-NIR) spectroscopy" untuk warna dan kandar gula buah tomat utuh segar telah dikembangkan dengan mengunakan analisis regresi "partial least squares" dengan metode "full cross validation". Model kalibrasi dikembangkan dengan menggunakan 150 sampel buah tomat. Model kalibrasi untuk warna tomat dikembangkan dengan menggunakan kisaran panjang gelombang dari 600~700 nm, sedangkan untuk kandar gula dikembangkan dengan menggunakan kisaran panjang gelombang dari 700~1098 nm. Koefisien korelasi (Rc2) dan kesalahan standar (SEC) dari kalibrasi untuk warna, masing-masing adalah 0.97 dan 0.15, sedangkan untuk kadar gula masing-masing adalah 0.96 dan 0.42 Brix. Model-model kalibrasi yang telah dikembangkan kemudian digunakan untuk memprediksi warna dan kadar gula buah tomat yang berasal dari satu set data secara terpisah, yang terdiri dari 104 sampel. Dalam pemprediksian warna tomat dihasilkan nilai-nilai koefisien korelasi, kesalahan standar, dan penyimpangan, berturut-turut adalah 0,92, 0,19 dan 0,09. Sedangkan untuk pemprediksian kadar gula berturut-turut adalah 0,91, 0,49 Brix, dan -0,04 Brix. Berdasarkan hasil ini disimpulkan bahwa "Vis-NIR spectroscopy" yang dilengkapi dengan kabel optic adalah salah satu metode yang sesuai untuk menentukan warna dan kadar gula tomat utuh segar. Jadi teknologi "Vis-Nir spectroscopy" dapat digunakan untuk mengklasifikasikan tomat segar ke dalam kelompok kualitatif yang didasarkan pada penampakan luar (warna) maupun tingkat kemanisannya (kadar gula).

Kata kunci : analisis nondestructive; near-infrared spectroscopy; regresi partial least squares; kualitas tomat.

INTRODUCTION

At the first time consumers buy fresh tomatoes is usually based on the appearance of fruit that correlated with fruit color, size or defects. Therefore, in post-harvest handling system, grading the quality of tomatoes is commonly based on the external appearance such as surface color, size or weight and defects. However, the frequency and amount of subsequent purchases is based largely on consumer assessment of eating quality such as flavor and texture. Therefore, it is necessary to grade the tomatoes based not only on external qualities but also on internal qualities such as sweetness.

Soluble solids content (SSC) is a major characteristic used to indicate an objective quality index in tomato, because the major component of SSC are sugar and organic acid that become an important contribution to the overall flavor of tomatoes. Bisogni et al. (1976) found correlation between SSC and sweetness, flavor and overall quality. Winsor (1966) reported that the best quality of fruit were those high in both sugars and organic acids.

To determine the SSC of tomatoes is normally performed destructively on juice using a refractometer. This method has two drawbacks, it requires the destruction of the sample and it is a time consuming. Near infrared spectroscopy has been used as a rapid and nondestructive methods for determining the quality of fruit and vegetable such as sugar in peaches (Kawano et al., 1992), dry matter of onions (Birth et al., 1985), SSC of cantaloupe (Dull et al., 1989), honeydew melon (Dull et al., 1992), fresh market tomato (Peiris et al., 1998), and apple (Murakami et al., 1994; Ventura et al., 1998; McGlone et al., 2002). However, the constituent concentration of fruit might be varies among the varieties and those might also influenced by the growing season. Therefore, the NIR studies should take account for variability of fruit compositions resulted from different harvesting time. This studies involved tomato samples collected from different harvesting time, from summer to autumn during 2 years. The objectives of this study were 1) to develop a nondestructive analysis method by using visible and near infrared (Vis-NIR) spectroscopy interfaced with fiber optic for determining the two important quality factors, color and SSC of intact tomatoes 2) to investigate the effects of different harvesting time on the accuracy of Vis-NIR prediction.

MATERIALS AND METHODS

Sample preparation

Tomato samples (Lycopersicon esculentum, cv. Maru) that had been grown in greenhouse in Chitose, Hokkaido were used in this experiment. In order to provide a wide range of constituent concentrations, tomato samples were selected from green maturity stage to red ripe stage. Tomatoes were sent directly to our laboratory in the same day after harvested. Picked samples are cleaned and before measurement, they were kept in an incubator at temperature of 20? for 24 h to make their temperature uniform. Tomato samples were collected during 2 years from 2001 to 2002. Samples collected in the first year from summer to autumn were used to develop a calibration model (150 samples) and those collected in the second year (104 samples) were used to validate the prediction accuracy of NIR calibration models.

Measurement of NIR spectra

All NIR spectra measurements were made with a Vis-NIR Spectroscopy (model 6500, NIR systems, silver spring MD) interfaced with fiber optic in combination with an IBM computer using the NSAS software program (Fig.1). To measure the optical absorption spectrum, each fruit is placed by hand on the center of probe (sensor) and in direct contact with the probe located inside the dark box. The spectra of tomatoes are recorded over the wavelength of 400-1100 nm region, at 2 nm intervals giving 350 absorbance points, by measure its transmittance. As an output, the spectra were expressed as absorbance (log 1/T) (T = transmittance). Prior to scan the samples, the first time is to make a scan reference using a Teflon block. The measurement of each spectrum was scanned 120 times. The spectrum of each fruit is measured at 4 different locations at around the equator of the fruit (between the blossom end and the stem end). The spectra from 4 equatorial locations of each fruit were averaged and the mean spectrum was deemed to be the spectrum of sample. After scanning, the color and SSC of each tomato was measured by using a standard method.

Standard measurement method

Surface color of each tomato was measured at 4 points on the shoulder. Color was measured with a reflectance colorimeter (Chroma Meter CR-200, Minolta Corp.) using the L* a* b* color system, where L* indicates lightness on a scale of 0 (= black) to 100 (= white), a* indicates green (-) to red (+), and b* indicates blue (-) to yellow (+). The color of each tomato is expressed as the ratio a*/b* to indicate the index color of the tomato, a higher a*/b* ratio indicating a redder surface color of the tomato.

The soluble solids content of the fruit was measured using a digital refractometer (PR-100). Each tomato was sliced in half. Each half was further divided into 3 parts, so there were 6 parts (replications) for each measurement per fruit. The juice from each part was extracted manually (> 2 drops) and put into the refractometer. The value of soluble solids content is expressed as %Brix.

Development and validation of NIR calibration models

The original NIR spectrum of each tomato sample was merged with standard data of color (a*/b* ratio) and SSC (oBrix), to perform a data set of calibration and validation. After all of spectra data were correlated with their constituents of interest, the calibration models were developed using the Unscrambler V. 6.11 software program with a partial least squares (PLS) regression analysis using a full cross validation method.

Calibration model of color was developed using the absorbance data over the wavelengths of 600 to 730 nm, and that of SSC was developed using the absorbance data over the wavelengths of 700 to 1098 nm. Calibration models of both color and SSC were established using 150 samples of calibration data set that collected during the first year and then each model was validated using a validation data set (115 samples) that collected during the second year. The predictive quality of the relationship between NIR spectra and standard data was evaluated using the correlation coefficient (R2), the standard error of calibration (SEC), the standard error of prediction (SEP) and the bias.

RESULTS AND DISCUSSION

The characteristics of tomatoes samples

The constituent concentrations of samples include surface color (a*/b* ratio) and soluble solids content (SSC) of 254 tomatoes were analyzed using a standard method. One set data of calibration is consists of 150 samples and that of validation is consists of 104 samples. Tomato samples were selected from green maturity stage to red maturity stage giving wide range of SSC and color index (a*/b* ratio). The SSC values of the data set of calibration was range from 3.79 oBrix to 11.39 oBrix with mean value and standard deviation were 6.66 oBrix and 1.57 oBrix, respectively, and that of the data set of validation was range from 4.19 oBrix to 10.58 oBrix with mean value of 6.81 oBrix and standard deviation of 1.71 oBrix, respectively. Surface color of tomatoes expressed as a*/b* ratio of the data set of calibration was range from -0.37 to 2.23 with mean value of 1.53 and standard deviation of 0.58, respectively. And that of the data set of validation was range from -0.18 to 2.23 with mean value and standard deviation were 1.58 and 0.49, respectively.

Changes of the NIR spectra of intact tomatoes

Changes of the absorbance (A) of each tomato at every wavelength were different that may correlated with the constituent of tomatoes. At a wavelength where the peak of absorbance take place is guessed have a relationship with the constituent of tomatoes. Therefore, the calibration models were developed from those wavelengths.

In order to know the differences among the absorbance spectra of different maturity stage of tomatoes, we selected green, pink, and red tomatoes in which each of them has the same soluble solids content (oBrix). The spectra are described in Fig. 2. At the wavelength of about 674 nm the peak of absorbance increased with a decreasing in a*/b* ratio. As explained above that a higher a*/b* ratio indicating a redder surface color of the tomato, and conversely a lower a*/b* ratio indicating a greener surface color of the tomato. Thus, the green tomato has an absorbance (log 1/T) higher than the pink and red tomatoes. Therefore, absorption band at wavelength of 674 nm was guessed has correlation with color of tomatoes. It was clear that by visual inspection of the original NIR spectra shows special characters of absorbance of visible radiation that could be used to quantitative measurements, and there were differences among the spectra of green, pink, and red color of tomatoes in the wavelength range of 600 nm to 730 nm. These wavelengths are the part of the electromagnetic spectrum that include in visible region. This result agrees with finding by Worthington (1974) who estimated the ripeness of externally green and red tomatoes on the basis of absorbance at wavelengths of 510 nm, 600 nm and 690 nm. Light absorbance was assumed to be due to chlorophyll in green tomatoes and carotenoids in red tomatoes (Watada, 1976).

The NIR spectra of intact tomatoes having low (3.79 oBrix), medium (6.80 oBrix), and high SSC (9.95 oBrix) are shown in Fig. 3. The original NIR spectra having different SSC values visually show clearly in absorption of NIR spectrum in the wavelength range from about 730 nm to 1098 nm. Another authors reported that wavelengths in the 900 to 920 nm range have been related to sugar content in onion (Birth et al., 1985) and peach (Kawano et al., 1992). However, the differences among the absorbance spectra of tomatoes having low, medium and high SSC were not as strong as like in the case of color (Fig. 1 and Fig. 2). When a number of wavelengths are selected in the regression model, various characteristics of the fruits are taken into account. In addition, as moisture content of tomatoes is high, more than 80% (wb), the absorption bands of SSC may be overlapping with the absorption bands of moisture content of tomatoes. It was known that water has absorption bands in the wavelengths of 760 nm, 970 nm, 1450 nm and 1940 nm (Osborne, 1986)

McGlone, V. A., Jordan, R. B., and Martinsen, P. J. (2002) Vis/NIR estimation at harvest of pre- and post-storage quality indices for 'Royal Gala' apple. Postharvest Biol. Tech. 25, 135-144.

Osborne, B.G.. and Fearn, T. (1988) Near Infrared Spectroscopy in Food Analysis. Longman Scientific & Technical, John Wiley & Sons, Inc.,6 05 Third Avenue,N ew York.

Peiris, K.H.S., Dull, G..G.., Leffler, L.G.. and Kays, S.J. (1998) Near-infrared (NIR) Spectrometric Technique for Nondestructive Determination of Soluble Solids Content in Processing Tomatoes. J. Amer. Soc. Hort. Sci.1 23(6),1 089-1093.

Ventura, M., Jager, A., Putter, H. and Roelofs, F. P.M.M. (1998) Non-destructive determination of soluble solids in apple fruit by near infrared spectroscopy (NIRS). PostharvestB iol. Tech.1 4,2 1-27.

Watada, A.E., Norris, K.H., Wortington, J.T., and Massie, D.R. (1976) Estimation of chlorophyll and carotenoid contents of whole tomato by light absorbance technique.J .F ood Sci.4 1,3 29-332.

Winsor, G..W. (1966) Some Factor Affecting the Composition, flavor and Firmness of Tomatoes.S ci.H ort.1 8,2 7-35.

Wortington, J.T. (1974) A light transmittance technique for determining tomato ripening rate and quality. Acta Hort. 1(38),1 93-195.

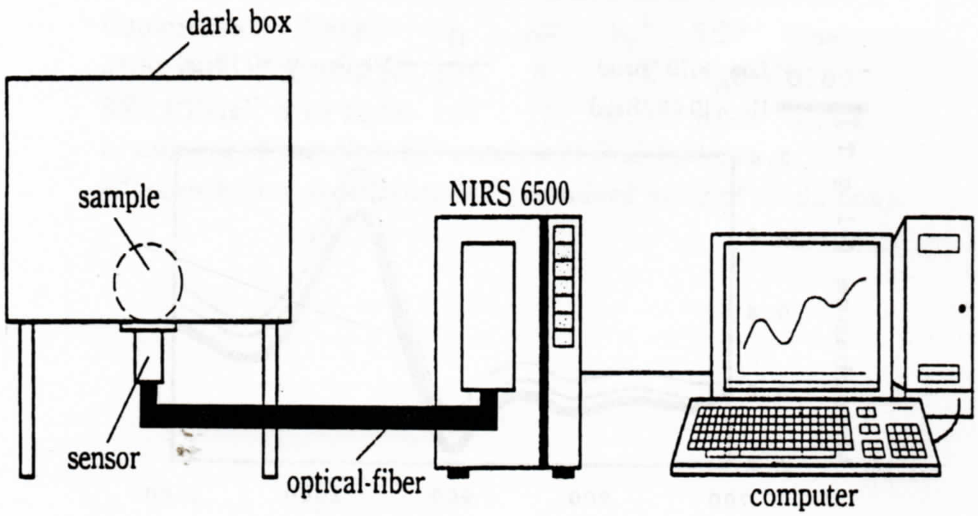

Fig.1. The measurement system of NIR instrument.

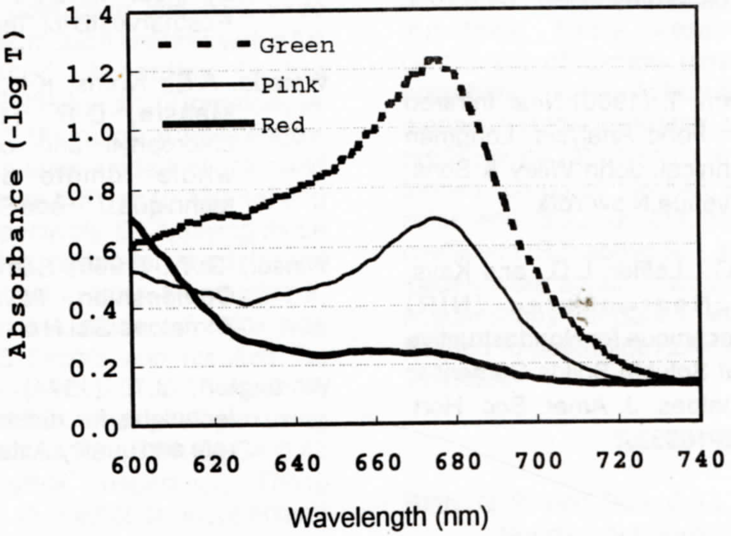

Fig. 2. Spectra of green, pink, and red tomatoes

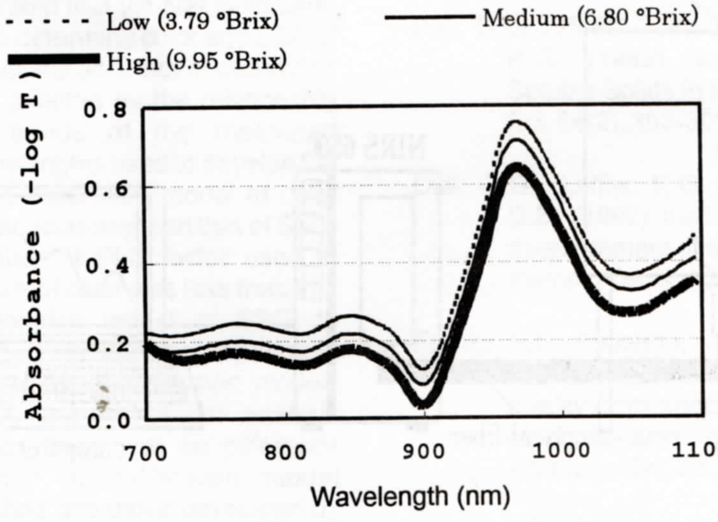

Fig. 3. Spectra of tomatoes having low, medium and high soluble solids content (SSC).

Table 1. Calibration models for Vis-NIR determination of color and SSC of tomatoes.

Constituent	Range	n	nF	R_c^2	SEC	Bias
a*/b* ratio	-0.37-2.23	150	3	0.97	0.15	0.00
SSC (°Brix)	3.79-11.39	150	10	0.96	0.42	0.00

n: number of samples; nF: number of PLS factors;
R^2: correlation coefficient; SEC: standard error of calibrations.

Table 2. Validation tests for Vis-NIR determination of color and SSC of tomatoes.

Constituent	Range	n	nF	R_p^2	SEP	Bias
a*/b* ratio	-0.18-2.23	104	3	0.92	0.19	0.09
SSC (°Brix)	4.19-10.58	104	10	0.91	0.49	-0.04

n: number of samples; nF: number of PLS factors;
R^2: correlation coefficient; SEP: standard error of predictions.