Nondestructive Determination of Soluble Solids in Tomatoes using Near Infrared Spectroscopy

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ABSTRACT

A nondestructive optical method for determining the soluble solids content of fresh whole tomatoes was investigated. The method, based upon near infrared spectrophotometric techniques, could predict the soluble solids content of tomatoes ($r = 0.92$, SEC = 0.27°Brix). Tomatoes from more than 30 popular fresh market cultivars at stages of maturity from mature green to ripe red fruit were studied.

Key Words: nondestructive, near infrared spectroscopy, soluble solids, tomatoes, maturity

INTRODUCTION

TOMATO FLAVOR QUALITY is a complex characteristic involving the perceived taste and aroma of numerous compounds (Stevens et al. 1977). Several researchers have found that the amount of sugars and acids and their interactions were highly related to flavor quality in tomatoes (e.g. Stevens et al. 1977, 1979). Hobson and Bedford (1989) found that taste panelists tended to dislike tomatoes with a deficiency in one or more of the major taste components (e.g., sweetness). Jones and Scott (1983) found that improvement in tomato flavor quality could be attained by increasing the sugar and acid content and concluded that breeding for tomato cultivars high in soluble solids content (SSC) was justified. Simandle et al. (1966) reported that taste panel scores correlated with SSC in tomatoes. Kader et al. (1977, 1978) showed that sweetness and ''tomato-like'' flavor were adversely affected by poor harvest and postharvest procedures such as early harvest or chilling.

Several researchers have attempted to use optical techniques to develop a nondestructive means of assessing tomato quality. The initial purchase decision by consumers is usually based upon appearance and the stage of ripeness is well correlated with fruit color. Thus, most optical systems have been developed to sense visible light characteristics of tomatoes associated with these attributes (e.g., Birth et al., 1957; Bittner and Stephenson, 1968; Nattuvetty and Chen, 1980; O'Brien and Sarkar, 1974; Worthington et al., 1976). Watada et al. (1976) used light transmittance through whole tomatoes to predict their carotenoid ($r = 0.97$ for lycopene, $r = 0.95$ for β-carotene) and chlorophyll ($r = 0.98$) pigment contents.

Near infrared (NIR) spectroscopy has been used as a rapid and nondestructive technique for measuring the soluble solids content (SSC) of several commodities. Dull et al. (1989) applied near infrared light at 884 nm and 913 nm to determine the SSC in cantaloupe. When the measurement was made on slices of cantaloupe the correlation between the NIR method and that determined by high-performance liquid chromatography was −0.97 with a standard error of calibration (SEC) of 0.56°Brix. When the measurement was made on intact cantaloupes the correlation dropped to −0.60 and the SEC increased to 1.67°Brix. Dull attributed some of the drop in correlation to light losses through the rind. Dull and Birth (1989) later refined their nondestructive method and applying it to honeydew melons improved the correlation between SSC and NIR measurement to −0.87, however the SEC was 1.6°Brix. Slaughter (1995) used a nondestructive NIR technique to predict the SSC of intact peaches and nectarines, $r = 0.92$ and SEC = 0.87°Brix. Kawano et al. (1993) used a calibration equation with 4 NIR terms to predict the SSC of intact satsuma mandarins, $r = 0.989$ and SEC = 0.28°Brix.

Traditionally, spectrophotometric methods use either direct transmission or diffuse reflectance geometries. These techniques are applicable where the optical path can be adjusted to minimize the sample's optical density or the composition of the sample's surface is the same as its interior. In nondestructive applications the sample is used in its natural, intact state frequently resulting in a high optical density which prevents the use of direct transmission and compositional differences between skin and interior which prevents the use of diffuse reflectance. For these cases researchers have developed a spectrophotometric technique termed ''interactance'' (Conway et al., 1988). Conway and others have used the term interactance because monochromatic light enters the fruit and ''interacts'' with the tissue inside. Some of the nonabsorbed light is internally reflected and exits the fruit on the same side as the entrance beam (as in Fig. 1). The interactance configuration allows the optical absorption spectrum to be collected from intact, optically dense biological specimens of irregular size such as tomatoes. This technique is similar to the ''body transmittance'' technique used by Birth et al. (1984), Dull et al. (1989), and Chen and Nattuvetty (1980).

Due to the high correlation between SSC and tomato flavor quality there is a need to rapidly and nondestructively determine SSC to assure that all tomatoes meet a minimum level of acceptance. Ideally such a system could determine the SSC of whole intact tomatoes without a priori knowledge of cultivar.

This research studied the feasibility of determining fresh whole tomato SSC with a nondestructive optical technique based upon NIR spectroscopy.

MATERIALS & METHODS

TOMATOES from more than 30 popular fresh market cultivars (including: Arletta, Better Bush, Celebrity, Early Girl, Heatwave, Jackpot, Sunny, Tango, etc.) were hand harvested in California at stages of maturity ranging from mature green to ripe red fruit. Ten replicate fruit of each of approximately six cultivars were tested weekly over a 7-wk period resulting in a total of 400 fruit for study. Some cultivars were included in the study twice, each time at a different maturity level, to guarantee a wide range of maturities. The tomatoes were stored at 15°C after harvest until ready to test and were equilibrated to room temperature (24°C) prior to evaluation.

The optical absorption spectrum from 400 nm to 1100 nm was measured at five different locations on each fruit using a fiber optic interactance probe (Fig. 1). The probe consisted of a central bundle of Schott glass fibers 7.6 mm in diameter surrounded by a 0.64 mm wide concentric ring of Schott glass fibers which had an outside diameter of 19 mm. The outer ring of fibers was separated from the central bundle by a 5.1 mm thick metal barrier. A rapid scanning (1.8 scans/sec) spectrophotometer (model 6500, NIR Systems, Silver Spring, MD) configured for interactance mode was interfaced to the fiber optic probe. At the spectrophotometer interface the fibers in the probe corresponding to the outer ring were reconfigured to align with the exit slit of the monoch-

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Table 1—Least Significant Difference (LSD) T test comparing the NIR SSC prediction error at different fruit locations

T grouping[b]	Mean | residual | (°Brix)	Std error (°Brix)	Fruit location[a]	
			Predicted	Calibrated
A	0.62	0.87	5	2
B	0.54	0.70	5	4
B				
B	0.54	0.70	5	1
B				
B	0.53	0.68	5	3
C	0.42	0.53	5	5
D	0.37	0.47	2	5
D				
E D	0.37	0.47	4	5
E D				
E D	0.37	0.48	1	5
E D				
E D F	0.36	0.45	3	5
E D F				
E G D F	0.34	0.43	4	3
E G D F				
E G D F	0.34	0.43	1	3
E G D F				
E G D F	0.34	0.43	4	4
E G D F				
H E G D F	0.33	0.43	2	4
H E G D F				
H E G D F	0.33	0.42	4	4
H E G F				
H E G F	0.33	0.42	2	3
H G F				
H G F	0.32	0.41	4	2
H G F				
H G F	0.32	0.41	4	1
H G				
H G	0.32	0.40	2	1
H G				
H G	0.31	0.41	3	4
H G				
H G	0.31	0.40	1	2
H G				
H G	0.31	0.39	2	2
H G				
H G	0.31	0.39	3	3
H G				
H G	0.30	0.38	1	1
H G				
H G	0.30	0.38	3	1
H				
H	0.29	0.37	3	2

[a] Fruit locations 1, 2, 3, and 4 represent equatorial fruit locations, location five represents the blossom end.

[b] Residual values with the same T Grouping letter are not significantly different (α = 0.05, LSD = 0.0425). Each grouping contains 400 observations.

rometer and those corresponding to the inner bundle were reconfigured to align with the silicon detector.

To measure the optical absorption spectrum, each fruit was hand placed on the probe so that the desired fruit location was centered on and in direct contact with the probe. The absorption spectrum was measured at each of five different locations on each fruit in a sequential manner. The first measurement was collected at a random location on the equator of the fruit. The next three measurements were taken on the equator at approximate 90°, 180°, and 270° rotations from the initial site. A fifth measurement was taken with the blossom end of the fruit centered on the probe. The average of 250 individual optical scans at each fruit location was stored for later use. A 20.8 mm thick Teflon® block was used as the optical reference standard for the system.

Following optical measurement the tissue from each fruit was comminuted in a blender for 60 sec. The soluble solids content of the comminuted tomato was determined using a temperature compensated refractometer. The optical and soluble solids data were then merged and a partial least squares (PLS, Martens and Naes, 1989) regression analysis was conducted using the NSAS software package (version 3.18, NSAS, 1990).

To determine any significant differences in the predictive ability of the five locations used for optical measurement, the data from each location were analyzed separately. Preliminary analysis using a trial and error process indicated that for the electro-magnetic region studied the wavelength range of 800 nm to 1000 nm would provide the best prediction of soluble solids content using the PLS multivariate calibration technique. PLS calibrations resemble principal component regression

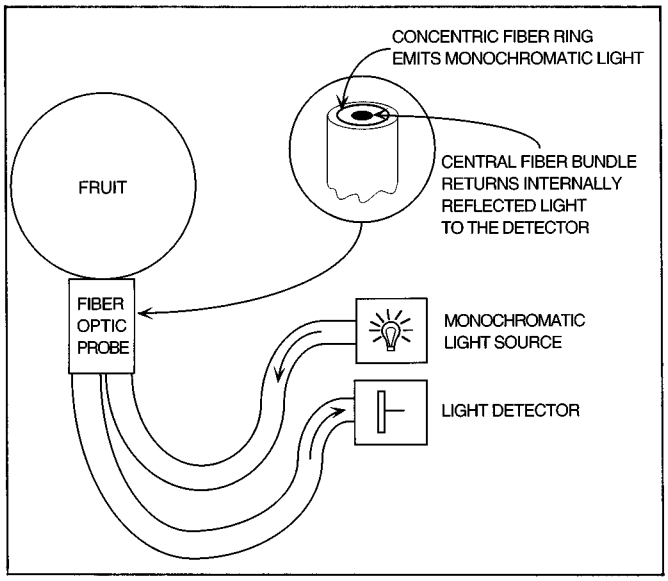

Fig. 1—Fiber optic configuration for light interactance measurements of intact fruit.

models in that regression factors are linear combinations of optical absorbance at each wavelength in the spectral region studied (i.e. 800 nm to 1000 nm). The correct number of regression factors for the PLS model was determined by the minimum mean square error of cross validation, where the calibration data set was split into four subsets of equal size (Martens and Naes, 1989). Cross validation of each of the five calibration models corresponding to the five different fruit locations indicated that as few as 6 PLS factors (for the blossom end location) to as high as 10 PLS factors (for one of the equatorial locations) could be used to predict the SSC. To facilitate direct comparison of the predictive ability of the five locations, five calibration models were developed, one for each location, each using six PLS factors.

Each calibration model was then used to predict the SSC of each fruit using optical data collected at each of the five locations. Residuals between the predicted SSC and the SSC determined by refractometer were calculated. This resulted in a total of 25 residuals for each of 400 fruit. A Fisher's LSD test was conducted on the absolute value of the residuals to determine if any calibration models were significantly better than others.

To determine the model with the best predictive performance, signal averaging was used to reduce random noise associated with fruit surface irregularity or fruit/probe placement. The optical data from the four equatorial locations was averaged for each fruit. To allow external validation of the calibration model this data set was randomly split into two subsets with the observations from 300 fruit reserved for model validation and the remaining 100 observations for model development (Neter et al., 1990). A PLS calibration was conducted using the cross validation technique previously described to determine the correct number of PLS factors. Once the calibration model was developed it was used to predict the SSC of each of the 300 fruit reserved for external validation.

RESULTS & DISCUSSION

THE AVERAGE ABSOLUTE VALUE of residuals and standard error values between the NIR predicted SSC and the SSC determined by refractometer were compared (Table 1). In general, it would be expected that the average residuals would be lowest when the calibration model developed at a particular location was used to predict the SSC using the optical information from that same location. Results indicate that all five calibration models (including that developed using data from the blossom end) had a significantly (α = 0.05) greater average residual when used to predict the SSC with optical data from the blossom end than from the four equatorial locations. The calibration developed at the blossom end had lower residual values when used to predict the SSC using equatorial data than from the blossom end data. The less reliable results obtained at the blossom end may have been due to physiological differences in the fruit at that location

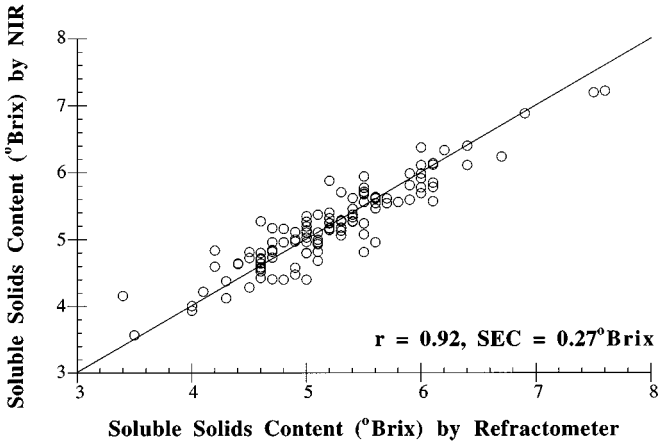

Fig. 2—Calibration results for nondestructive prediction of soluble solids content.

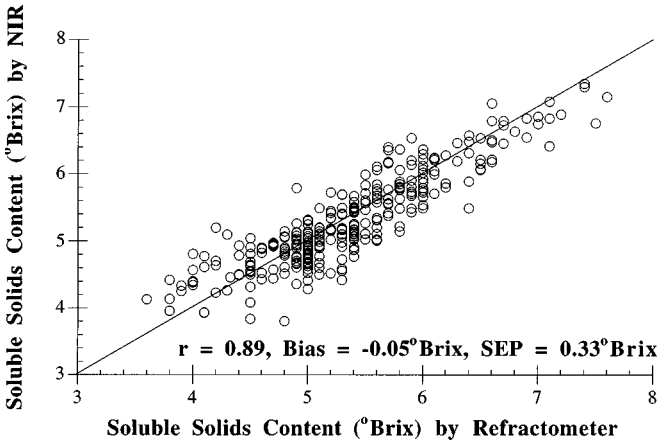

Fig. 3—Validation results for nondestructive prediction of soluble solids content.

and requires further study. These results indicate that the blossom end should be avoided when attempting to predict SSC using the NIR technique employed here.

The residual values from the four equatorial locations did not indicate consistent differences between the calibrations developed with optical data from these four locations. The standard error of prediction (SEP) for SSC ranged from 0.29°Brix to 0.43°Brix when the calibration developed at one equatorial location was used with optical data from a different equatorial location on the same fruit.

A PLS calibration analysis was conducted to predict the SSC of 100 randomly selected fruit (based upon the average NIR data of four equatorial locations of each, Fig. 2). Cross validation indicated that a calibration model using 12 PLS factors was appropriate, r = 0.92 and SEC = 0.27°Brix. Validation results were obtained from application of the calibration model to the remaining 300 tomatoes (Fig. 3). The validation data had a correlation coefficient of r = 0.89, a SEP of 0.33°Brix with a bias of -0.05°Brix. These results indicate that use of 12 PLS factors did not lead to overfitting and that the calibration model appeared to be valid. The SEP value based upon an average optical reading from four different equatorial positions was smaller than any of the SEP values shown (Table 1).

CONCLUSIONS

NIR SPECTROSCOPIC TECHNIQUES can be used to nondestructively determine soluble solids content of intact tomatoes. The interactance technique had significantly greater accuracy when used at a random position along the equator of the fruit than at the blossom end. In developing high speed sorting equipment for SSC, orientation of the fruit to allow measurement on the fruit equator would be recommended.

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