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Comparison of detection modes in terms of the necessity of visible region (VIS) and influence of the peel on soluble solids content (SSC) determination of navel orange using VIS–SWNIR spectroscopy

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ABSTRACT

Comparison of three detection modes (interactance, reflectance and transmittance) was performed in terms of the necessity of visible (VIS) region and the interference caused by peel in SSC assessment of navel oranges. Spectra of 88 oranges with peel and peeled were collected using a commercial available CCD spectrometer. Partial least squares (PLS) regression was used to develop calibration models. Results showed that the participation of VIS region degraded the performances of PLS models in transmittance mode, while for the other two modes VIS–SWNIR models turned out to be the best. The peel of oranges did not bring about significant negative influence on SSC determination in any detection mode. The best calibration models were achieved with transmittance mode regardless of sample status. Future research should be focused on specific reasons such as the composition of orange peel and the influence of different sizes of fruits.

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1. Introduction

Over the years, with the improvement of living standard, consumers' attention to fruits' quality is not limited to external appearance, but further extends to internal quality represented by soluble solids content (SSC) which has been proved to have good correlations with consumers' acceptance of fruits like mandarin (Cayuela, 2008). Mandarins belong to a wide range of citrus fruits that also include oranges (among them Valencia and navel orange), grapefruit, lemon, etc. They are all characterized by relatively thick peel, abundant juice, easy-to-peel rind and segments that separate easily (Sánchez et al., 2013). The SSC of mandarin is mostly related to the stage of ripeness and is always utilized as one critical internal quality indicator of mandarin.

Near infrared (NIR) spectroscopy is thought to be one of the most appropriate techniques for fast assessment of fruits' internal quality. Recently, with the availability of charge coupled device (CCD) detectors, the utilization of visible-near infrared (VIS-NIR) spectroscopy in measuring fruits' internal quality has made a great progress, including quality detection in citrus fruit (Antonucci et al., 2011; Cayuela, 2008; Cayuela and Weiland, 2010; Gómez et al., 2006; Jamshidi et al., 2012; Sánchez et al., 2013). The researches listed above were mostly accomplished with the

visible-shortwave near infrared (VIS–SWNIR) spectroscopy. In the study of Li et al. (2013), the authors pointed out that the best prediction results were obtained with the participation of the VIS region. However, the studies of Fernández-Novales et al. (2009) and Subedi et al. (2007) indicated that the use of SWNIR without VIS region was also able to generate good results. Chia et al. (2013) compared the performances of SWNIR and VIS–SWNIR models for assessing SSC of pineapple in reflectance mode. Results indicated that VIS region did not provide unique relevant information. But their study was just based on diffuse reflectance mode. Hence, it is not clear whether the conclusion is true for other modes (transmittance, reflectance). So it appears that the involvement of VIS region in SSC determination should be further investigated.

Citrus fruits often possess relatively thick peel, which may interfere the nondestructive determination of internal quality using VIS–NIR spectroscopy. Fraser et al. (2003) studied light distribution inside mandarin fruit during internal quality assessment by NIR spectroscopy. It was found that the skin of mandarin created a significant internal reflection leading to elevated light level in the fleshy part, thus influencing the scatter and absorption of light. Shi et al. (2010) found that peel led to significant influence on the calibration model of apple firmness with diffuse reflectance spectroscopy. In a review concerning NIR spectroscopy applications for internal and external quality analysis of citrus fruit, Magwaza et al. (2012) argued that for thick peel fruit, the



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distorting influence of peel was more pronounced. Considering the penetration ability of light, the interference caused by peel should be considered in different detection modes.

The objectives of this study were (1) to evaluate the necessity of VIS region in SSC assessment under three detection modes; (2) to analyze the interference caused by peel in SSC assessment under three detection modes; and (3) to achieve the best calibration model after the comparison of three spectrum acquisition modes based on step (1) and (2).

2. Materials and methods

2.1. Fruit samples and experimental procedures

In the present work, a total of 110 Sunkist navel oranges were purchased in local market. In order to guarantee the uniformity of size and weight, 88 navel oranges were selected manually. All samples were individually washed, dried, and numbered. For each sample, three circles (named 1, 2, 3) were marked around the equator (120°). All experiments were accomplished in laboratory environment whose temperature and relative humidity were set to constant (temperature: 20 °C, relative humidity: 50%), in order to prevent the influence of temperature fluctuation on VIS-NIR spectra (Yao et al., 2013; Zude-Sasse et al., 2002). The specific experimental procedures were: (1) the maximum equatorial diameter and height (length from stem to blossom end) of each intact orange were measured using a digital caliper, and each weight was determined with an electronic balance; (2) spectra of all intact oranges were collected in three detection modes (reflectance, transmittance, interactance) at the locations marked (1, 2, 3); (3) peel of all navel oranges were removed with the help of a peeler, three new circles were marked on the flesh at the same place before the peel was removed; (4) step (1) was repeated for all peeled oranges; (5) step (2) was repeated for all peeled oranges and peels; and (6) all peeled oranges were juiced using a squeeze juicer, the SSC of each orange was measured by a digital refractometer (model PR-101, Atago Co., Ltd., Tokyo, Japan) after the juice was filtered.

2.2. Spectroscopy

All measurements were performed with a commercially available VIS–SWNIR CCD spectrometer (Model QE65000, Ocean Optics Inc., USA), which was equipped with a back-thinned silicon detector (200–1100 nm) and a thermal electronic cooler to alleviate temperature change of detector and improve the signal-to-noiseratio (SNR). For transmittance measurements, the apparatus (Fig. 1(a)) used was similar with the Mode T4 applied in the research of Fan et al. (2009). Two tungsten halogen lamps (100 W, 12 V) were arranged at a distance of about 200 mm from the orange surface, the angle between the lamp and the horizontal line was 45°, the axes of the two lamps were perpendicular to each other. A piece of black sponge (5 mm thickness) with a 30 mm hole was attached between fruit and fruit holder, acting as a light seal and a flexible support to accommodate different oranges.

With respect to diffuse reflectance mode (Fig. 1(b)), the light source was a light source module (20 W, 24 V, model HL-2000-HP, Ocean Optics Inc., USA) which covered the spectrum ranging from 360 nm to 2000 nm. A bifurcated optic fiber cable that enclosed light source beams and receptor beams randomly was applied to direct light emitted by light source and to receive the light signal which was reflected by samples.

For interactance mode (Fig. 1(c)), a fiber optic ring light guide similar to that used by Kavdir et al. (2007) was applied to irradiate samples. The detector probe was installed in the center of the ring light guide to catch light signal. The light source was a tungsten halogen lamp (100 W, 12 V).

Before collecting spectra of samples, dark spectrum and reference spectrum was measured and stored after light source was stabilized. Each sample was placed centrally and steadily on the black sponge manually, with stem-calyx axis horizontal, for transmittance mode, stem-calyx axis of sample was also perpendicular to the plane consisting of two lamp axes. Three spectra were obtained for each sample with three circles facing the detector respectively in any detection mode.

2.3. Chemometrics and data analysis

The three spectra of every sample were averaged into one for further analysis. The overall mean spectra of all samples were then converted to absorbance values $(\log(1/T), \log(1/R))$ to obtain linear correlation between spectra and sample molecular concentration (Jamshidi et al., 2012; Liu et al., 2008; Shao et al., 2007). For spectra obtained from different modes, the beginning and end with different regions were ignored because of the existence of pronounced noise. Thus, the spectrum regions to be used were: 520-1000 nm for interactance, 460-1000 nm for reflectance, 550-930 nm for transmittance. To analyze the necessity of VIS region, the wavelength 700 nm was chosen as demarcation point, considering that there was not any organic molecules absorption below 700 nm (Bamfield and Hutchings, 2010; Walsh et al., 2000). This division of wave band was in accord with that described in other publications (Cayuela, 2008; Chia et al., 2013; Magwaza et al., 2012; Pellicer and Bravo, 2011).



Fig. 1. General sketches of transmittance, reflectance mode and interactance mode. (1) Light source; (2) navel orange; (3) black sponge; (4) fruit holder; (5) spectrometer; (6) fiber; (7) bifurcated optic fiber; and (8) ring light guide.

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