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Fourier transform near infrared diffuse reflectance spectroscopy and two spectral acquisition modes for evaluation of external and internal quality of intact pomegranate fruit

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ABSTRACT

Fourier transform near infrared (FT-NIR) diffuse reflectance spectroscopy as a non-destructive method for the development of calibration models has been investigated as a means of assessing the quality of whole pomegranate fruit. FT-NIR diffuse reflectance spectrometers with different spectral acquisition modes were evaluated using direct contact between the sample and the integrating sphere (IS), or by a contact-less measurement using an optic fibre coupled emission head (EH) to scan fruit over a distance of 170 mm. Fruit weight, firmness and colour components (a*, Chroma, hue angle), total soluble solids (TSS), pH, titratable acidity (TA), sugar to acid ratio (TSS:TA), BrimA, total phenolics, total anthocyanin and vitamin C. The best prediction statistics obtained from calibration models of the EH were firmness (R^2 = 83.0, residual predictive deviation (RPD) = 2.43), fruit colour components (a*: R^2 = 90.9, RPD = 3.34); Chroma: R^2 = 83.0, RPD = 2.43, TSS (R^2 = 78.1, RPD = 2.17), TA (R^2 = 76.8, RPD = 2.12), BrimA (R^2 = 76.2, RPD = 2.08), total phenolics (R^2 = 88.0, RPD = 2.91) and vitamin C (R^2 = 76.2, RPD = 2.06). The best prediction obtained from calibration models of IS were colour component Hue (R^2 = 83.9, RPD = 2.50), TSS:TA (R^2 = 86.8, RPD = 2.72) and total anthocyanin (R^2 = 62.6, RPD = 1.64). Overall, good prediction was observed for both the EH and IS; however, better prediction performance was obtained with the EH which gave the best prediction for 9 of the 13 quality parameters evaluated. These findings have demonstrated that the EH (a contactless option of the Matrix-F) can be implemented as an online tool for the analysis of pomegranate fruit quality.

1. Introduction

External quality evaluation of pomegranate fruit is based on the measurement of parameters such as fruit weight, rind colour and firmness. Internal fruit quality related to organoleptic aspects include total soluble solids (TSS), titratable acidity (TA), TSS:TA ratio and total phenolic content. Traditional method of measuring these internal quality attributes are destructive in nature, require specialised sample preparation, labour intensive and inapplicable during grading and sorting in commercial packing operations. Moreover, fruit quality determined destructively may display significant variation due to difference in maturity, growing region and fruit canopy position (Magwaza et al., 2013). In order to supply high quality fruit to the international market, an alternative non-destructive approach is required.

Near infrared (NIR) spectroscopy is a non-destructive technique that interacts with molecular groups which consist of C—H, O—H and N—H bonds providing information about the proportion of each including scattering from microstructures which can be indirectly related to physical properties (Nicolaï et al., 2007). Furthermore, NIR is regarded as one of the most advance in chemometric software packages and commercial application (Nicolaï et al., 2007; Magwaza et al., 2012). Published NIR based research on different quality attributes for pomegranate fruit is limited to one study. Khodabakhshian et al. (2016) focused on the use of Vis/NIR for the measurement of sugar and acidity

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content. However, several key parameters used to evaluate pomegranate quality still needs to be assessed such as fruit weight, fruit colour, firmness, TSS:TA ratio and more recently BrimA (Fawole and Opara, 2013a). BrimA index is a variant of TSS/TA and a criterion for acceptance of fruit juice, relating to the sensory properties of the fruit. The index allows smaller amounts of acid than sugar to make the same numerical change to BrimA (Fawole and Opara, 2013b). Therefore, evaluation of these parameters could contribute to the implementation of suitable management strategies to predict and control desired pomegranate quality attributes. Furthermore, the pomegranate is a rich source of vitamin C and several other active polyphenolic compounds (Viuda-Martos et al., 2010; Ismail et al., 2012; Opara et al., 2009). Accurate and reliable prediction of these chemical constituents during postharvest handling and processing could contribute in providing high quality fruit rich in vitamin C and phytochemicals to consumers.

In industrial applications, conventional spectrometers can only be installed close to the stage where the product such as fruit is measured, whereas the fibre optic probes make it possible to reach measurement points that are difficult to access. The application of FT-NIRS in process control has potential for on-line analysis of fruit quality. The objective of this study was, therefore, to evaluate two different spectral acquisition modes; direct contact between the sample using a rotating integrating sphere (IS) and a contact-less measurement using an optic fibre coupled emission head (EH) for the prediction of external and internal quality parameters of intact pomegranate fruit. The contactless option simulates the situation in the pack-house for online application, whereas direct contact provides an ideal tool to meet the requirements for research applications.

2. Materials and methods

2.1. Fruit supply

This research was carried out during the 2015 season using pomegranate (cv. Wonderful) procured from two commercial orchards in the area of Western Cape province, South Africa (33°34′851″S, 19°00′360″E). A total of 200 fruit was obtained from Heinrich Frederich Schaefer (HFR) orchard, while another set of 100 fruit was obtained from Porterville to add orchard location variability. The fruit were transported to the Postharvest Technology Research Laboratory at Stellenbosch University. On arrival, fruit were equilibrated at ambient conditions before being sorted for size uniformity.

2.2. Spectral acquisition

Two different spectral preselection methods were used to obtain NIR spectra of the fruit; the Multi-Purpose Analyzer (MPA) FT-NIR spectrophotometer (Bruker Optics, Ettlingen, Germany) and MATRIX™-F FT-NIR spectrophotometer (Bruker Optics, Ettlingen, Germany). NIR spectral data were acquired on opposite equilateral sides of each fruit over a spectral wavelength range of 800–2500 nm. The acquired spectra for each fruit were averaged to obtain a single spectrum. During NIR spectral acquisition the same fruit samples were measured sequentially using two different spectral acquisition methods at room temperature. The MPA was equipped with an IS for direct contact with the sample and measure diffuse reflectance. Fruit samples were placed on a 50 mm width accessory sample holder which is used for measurement of highly scattering solid media. The MPA is equipped with a permanently aligned and highly stable RockSolid™ interferometer which consist of gold coated mirrors with a beam splitter which is made of a quartz substrate (Magwaza et al., 2013). The NIR beam is directed into the gold coated sphere and through the centre of the sphere into the pomegranate sample. Due to the gold coating, the reflected light re-enters the sphere and are collected and directed towards the detector. The integrating sphere uses a PbS detector with nonlinearity correction. The wavelength range scanned was from 800 to 2500 nm (12500–4000 cm^{-1}) with a scanning resolution of 8 cm^{-1} and scanner velocity of 10 kHz. For each spectrum a total of 128 scans were acquired which averaging about 120 s per sample and after 30 min reference measurements were performed against air background.

The MATRIX™-F (Q410/A) FT-NIR spectrometer was equipped with a fibre optic EH (230 mm diameter, 185 mm height and 170 mm focus depth) mounted 185 mm above the sampling platform for contactless measurement of the fruit. The EH contains 4 air cooled tungsten NIR light sources (tungsten halogen, 12 V, 20 W). The diffused reflected light was collected via an optic fibre cable connected to the spectrometer which is equipped with a thermoelectrically cooled and temperature-controlled TE InGaAs diode detector. Prior to scanning fruit, reference measurements were taken against air background and periodically at intervals of 30 min between measurements. The wavelength range, scanning resolution and a number of scans per spectrum were the same as the MPA FT-NIR spectrophotometer. In both instruments, the measurement the NIR spectra system was operated was achieved using OPUS software (OPUS v. 7.0 for Microsoft, Bruker Optics, Ettlingen, Germany). Illustration of the two different spectrometers is presented in S1.

2.3. Reference measurements

The weight of each fruit was determined using an electronic scale (Mettler Toledo, Model ML3002E, Switzerland, 0.01 g accuracy). A fruit texture analyser (GÜSS-FTA, South Africa) fitted with a cylindrical probe (5 mm) which was used to measure fruit firmness. Rind colour components were performed using a calibrated colour Chroma Meter (CR-400 Minolta Corp, Osaka, Japan). Chroma (C*) and Hue angle (h°) was derived from the colour components L*, a*and b* as described by Pathare et al. (2013): Individual fruit were manually peeled and the extracted arils were juiced using a Liquafresh juice extractor. The juice was filtered through a 1 mm sieve and immediately used measure the TSS, pH and TA and the remainder of the juice was stored in a freezer (VF720 −86, SNIJDER LABS, Netherlands) at −80 °C for further analysis of phytochemicals and vitamin C concentration.

A hand held digital refractometer was used to assess the percentage of total soluble solids within the juice. A titrosampler (Metrohm, Switzerland) was used to assess the acidity (citric acid%) by titration of 2 mL fresh juice against 0.1 M NaOH solution. To ensure that samples of both orchards had sufficient variation in TSS and TA, their distribution frequency was assessed. Pomegranate fruit samples (n = 300) were categorised into four groups (high TSS high TA, high TSS low TA, low TSS high TA and low TSS low TA) according to Arendse et al. (2017). The distribution frequency of the variation in TSS and TA in pomegranate fruit samples (n = 300) are presented in Fig. 1. The sample collection showed a wide range of variability in TSS and TA within the sample set. The pH values were determined using a calibrated pH meter (Crison, Model 924, Barcelona, Spain). The sugar to acidity ratio was

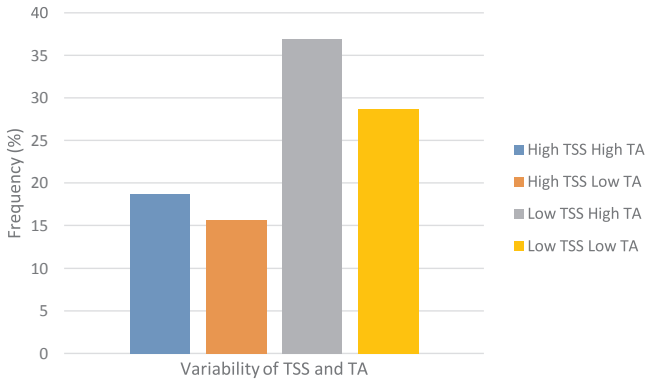

Fig. 1. Sample frequency (%) vs variability of TSS and TA for pomegranate fruit samples (n = 300) with high TSS ≥ 15% and high TA ≥ 1.5%.