



# A comparative study of reflectance and transmittance modes of Vis/NIR spectroscopy used in determining internal quality attributes in pomegranate fruits

Rasool Khodabakhshian<sup>1</sup> · Bagher Emadi<sup>1</sup> · Mehdi Khojastehpour<sup>1</sup> · Mahmood Reza Golzarian<sup>1</sup>

Received: 12 December 2018 / Accepted: 24 July 2019  
© Springer Science+Business Media, LLC, part of Springer Nature 2019

## Abstract

The objective of this study was to compare transmission and reflectance modes of visible (VIS)/near infrared (NIR) spectroscopy for their ability to nondestructively determination of key pomegranate quality attributes such as total soluble solid content (TSS), pH and firmness. Partial least squares (PLS) regression was used to develop calibration models. The reflectance mode predicted TSS with  $r=0.95$ ,  $RMSEC=0.22$  °Brix and  $RPD=6.7$  °Brix by calibration models. These parameters for the validation models were found to be:  $r=0.94$ ,  $RMSEP=0.21$  °Brix and  $RPD=6.72$  °Brix. The pH was predicted with  $r=0.85$ ,  $RMSEC=0.068$  °Brix and  $RPD=4.58$  °Brix for calibration set and  $r=0.86$ ,  $RMSEP=0.069$  °Brix and  $RPD=4.43$  °Brix for validation sets by reflectance mode. The results indicated that it was possible to use both the transmission and reflectance modes to develop a system in determination of the internal attributes of pomegranate fruit. However, reflectance mode spectra provided more accurate assessment of TSS, pH and firmness.

**Keywords** Fruit quality · Pomegranate · Vis/NIR spectroscopy · Reflectance · Transmittance

## Introduction

Nowadays, with the improvement of standard of living, the fruit industries such as pomegranate industry have been immensely thrived to provide the consumers with products of high internal quality [1, 2]. Pomegranate (*Punica granatum L.*) fruit is one of the economically important fruits which is eaten both as fresh fruit and in processed forms such as juice, jelly or jam all over the world. In most countries that produce pomegranate fruit, the bulk of pomegranate is consumed in fresh form [1]. Therefore, in line with the recent general concerns for food quality and safety, many technologies for assessing the quality of fresh pomegranates are being investigated. Most instrumental techniques used to measure internal quality of pomegranate are destructive in nature and involve a considerable amount of manual work [2, 3]. Thus, to ensure the minimum acceptability of the fruits quality to consumers, it is important to develop efficient

and nondestructive methods to measure internal attributes of pomegranate fruit.

In recent years, many research works have been conducted worldwide to develop nondestructive methods to assess fruit qualities. NIR spectroscopy has proven to be a promising method for determination of the internal quality of agricultural products such as apple [4], apricot [5], avocado [6], banana [7], cherry [8], citrus [9], grape [10], jujube [11], kiwifruit [12], mandarin [13], mango [14]; peach [15], pear [16], pepper [17], plum [18], pineapple [19], pomegranate [20, 21], watermelon [22], and tomato [23]. The captured radiation spectra has been demonstrated to be related to the physical structure as well as the chemical composition of the product matrix [24].

However, application of the technique varies and there are three standard measurement modes for the acquisition of NIR spectra from a sample: transmission, reflection and interactance. Some researchers have used reflectance mode, where it measures the light backscattered from the surface of an object [8, 24–28]. Some studies have been conducted on transmission mode, which the light is pointed at one side of an object and normally the signal is collected from the other side [29–31]. Interactance, which is sometimes also called ‘partial light transmittance’, has been used by some

✉ Rasool Khodabakhshian  
khodabakhshian@um.ac.ir

<sup>1</sup> Department of Biosystems Engineering, Ferdowsi University of Mashhad, Mashhad, Iran

researchers [30–33]. Interactance is a mode where a light seal separates the field of view of the detector from the illuminated fruit surface.

Based on the previous studies, each of three mentioned modes of near infrared spectroscopy can be used to determine internal quality attributes. However, it seems that transmission mode could provide better assessment of fruit internal quality. In the reflectance mode, the acquisition of spectra is easier and intensity levels are relatively high. However, this mode may be more susceptible to variations in shallow subsurface or on-surface properties of the fruit; in transmission mode may be less susceptible to surface properties, but there is a reduced signal-to-noise ratio due to very small amount of light penetrating into the flesh [34]. This makes it difficult to obtain accurate transmission measurements at grading line speeds, particularly where high ambient light exists. Interactance mode can resolve the issues associated with reflection and transmission modes in each of these characteristics. However, obtaining a light seal in this mode is still a challenge at the high conveyor speeds used in modern fruit grading systems.

In spite of these uncertainties there have been few studies that directly compared the merits of the different measurement modes [33–36]. Also among these papers only Schaare and Fraser (2000) compared the different measurement modes used in the assessment of fruit internal quality [33]. Therefore, the objective of this study was to compare the performance of reflectance and transmission modes of Vis/NIR spectroscopy to predict internal quality attributes (TSS, pH and firmness) of pomegranate fruit in a nondestructive manner.

## Material and methods

### Sample preparations

Pomegranate fruits (ASHRAF variety) for this study were harvested from an orchard in Shahidabad Village, Behshahr County, Mazandaran Province, Iran during commercial harvest time (October 2014) (Fig. 1). A total of 100



**Fig. 1** Fruit and arils of pomegranate (cv. ‘ASHRAF’) cultivar

pomegranate fruits without any damage were selected for this study. Samples were washed, dried, and labelled, and the morphological properties of each sample (including fruit length without calyx (L), expressed in mm; fruit width (W), expressed in mm; fruit thickness (T), expressed in mm; geometric mean diameter,  $D_g$  (mm); sphericity,  $\phi$ ; surface area, S (mm<sup>2</sup>); volume, V (cm<sup>3</sup>) and fruit mass, expressed in g) were measured and recorded before spectroscopic measurements using the methods introduced by Mohsenin [37]. The results are shown in Table 1. Then, the samples were randomly divided into two subgroups. The first subgroup of 70 samples was used as a training set for developing partial least square (PLS) model. The remaining subgroup of 30 fruits was used for model validation and to verify the prediction power of the predictive models. All pomegranate samples were measured using reflectance, and transmission spectroscopy after 2 days of equilibration at 20 °C and 60% relative humidity. Following spectral measurements, the internal quality attributes (TSS, pH and firmness) of samples were determined.

### TSS, pH and firmness measurements

In order to assess the real quality attributes of pomegranate fruit, the TSS, pH and firmness were determined using traditional destructive tests. Firmness measurement of samples was made using an Instron Universal Testing Machine (Model H5KS, Tinius Olsen Company, U.S) with a 5 mm cylindrical probe programmed to penetrate 8 mm into test fruits at the speed of 10 mm/s. Duplicate puncture tests were performed on opposite sides of equatorial region of each fruit and average value was reported. Peak force required to puncture fruit skin was taken as fruit firmness. Then the samples were macerated with a commercial juice extractor, filtered and centrifuged afterwards. The total soluble solid content (TSS) and pH of juice were measured thrice using a

**Table 1** Morphological properties of the samples

Attributes	Max	Min	Mean	SD
L (mm)	66.28	62.03	64.02	2.13
W (mm)	73.15	67.14	70.15	3.05
T (mm)	69.84	68.82	67.12	2.6
$D_g$ (mm)	68.25	64.15	66.95	2.13
$\phi$	0.96	0.94	0.95	0.01
S (mm <sup>2</sup> )	14,782.63	13,675.42	14,081.57	872.13
V (cm <sup>3</sup> )	162.35	151.54	157.20	6.72
Fruit mass (g)	166	153	160	8.12
Fruit firmness (N)	41.97	38.5	61.38	1.63
Total soluble solid (°Brix)	19.2	18.42	18.64	0.32
pH	3.65	3.42	3.51	0.11

hand-held refractometer (TYM Model, Mettler Toledo Company, China) and a digital pH meter (3020 Model, JenWay Company, U.K) respectively, and the average values were noted. All experiments were performed in same conditions.

### Spectral acquisition

From each fruit, four spectra (400–1100 nm at intervals of 1 nm) in reflectance and transmission modes were collected at four equidistance positions along the equator using a dual-channel spectrometer (AvaSpec-2048TEC, Avantes Company, Netherlands) equipped with an AvaSoft7 software, 1 nm resolution and sensitivity of 2000 count per 1 mJ entrance irradiation. The light source used for both reflectance and transmission modes was a tungsten halogen lamp (100 W, 12 V) that could be used in both the visible and near-infrared regions. Under reflectance (transmission) mode, the light source was arranged at a distance of about 15 cm from the fruit surface and the angle between the incident light source and the fiber optic (that guide reflectance light to a detector) was set to 45°. Under transmission mode, the halogen lamp was placed at an angle of 90° to the fiber optic. A white Teflon material was used as the reference material before every measurement. Dark current was measured automatically prior to each measurement. The integration time was set 50 ms.

### Qualitative chemometric analysis

In order to obtain reliable, accurate and stable calibration models, the raw data acquired from spectrometer need to be preprocessed first to reduce the effect of irrelevant information such as background and noise spectra [38–40]. In this study, the pretreatments were implemented by ParLeS software version 3.1 [41]. Firstly in this study, four spectra of every sample were averaged into one spectrum and then converted to absorbance value to obtain linear correlation between spectra and sample molecular concentration. Finally, different preprocessing methods including centering, smoothing by Savitzky–Golay algorithm, median filtering, normalization (Multiplicative Scatter Correction, MSC and standard normal variate, SNV) and differentiation (first derivative and second derivative) were performed.

Partial least squares (PLS) regression method was used to fit a model on spectral responses (average spectra with 700 wavelengths in the range from 400 to 1100 nm) from samples and their quality attributes (TSS, pH, or firmness) was. When applied to spectral of the calibration set (70 samples), the aim of PLS analysis was to find a mathematical relationship between a set of independent variables,  $X$  matrix ( $N_{70\text{fruits}} \times K_{700\text{wavelengths}}$ ), and the dependent variable,  $Y$  matrix ( $N_{70\text{fruits}} \times 1$ ). The values of each attribute (TSS, pH, or firmness) from the calibration set were used

to represent the dependent variables ( $Y$ ). Meanwhile, the spectral values at 700 wavelengths of the 70 pomegranate fruits represented the independent variables or the predictors ( $X$ ). The remaining data associated with the 30 sample fruits were randomly allocated for validation. Spectral and concentration residuals showed that there was no outlier in all datasets. The optimal number of latent factors for establishing the calibration model was determined using the minimum value of predicted residual error sum of squares (PRESS). The performance of model calibration and validation was presented in terms of correlation coefficient ( $r$ ), root mean square error of calibration (RMSEC), root mean square error of prediction (RMSEP) and ratio performance deviation (RPD) as follows [42]:

$$r = \sqrt{\frac{\sum_{i=1}^n (\hat{y}_i - y_i)^2}{\sum_{i=1}^n (\hat{y}_i - y_m)^2}} \quad (1)$$

$$RMSEC = \sqrt{\frac{1}{n_c} \sum_{i=1}^{n_c} (\hat{y}_i - y_i)^2} \quad (2)$$

$$RMSEP = \sqrt{\frac{1}{n_p} \sum_{i=1}^{n_p} (\hat{y}_i - y_i)^2} \quad (3)$$

$$RPD = \frac{SD}{RMSEC(P)} \quad (4)$$

where  $\hat{y}_i$  is the predicted value of the  $i$ -th observation,  $y_i$  is the measured value of the  $i$ -th observation,  $y_m$  is the mean value of the calibration or prediction set,  $n$ ,  $n_c$ , and  $n_p$  are the number of observations in the data set, calibration set and prediction set, respectively. Generally, a good model should have higher correlation coefficients; lower both RMSEC and RMSEP values, but also a small difference between RMSEC and RMSEP or a RPD value should be more than 5 [43].

## Results and discussion

### Morphological properties of the samples

Table 1 shows the summary statistics and variations in morphological properties of samples including the range of fruit mass and the three main dimensions. As can be seen in this table, the samples varied in terms of morphology. Therefore, the variation was the main reason to use normalizing preprocessing methods (MSC and SNV) and correct the multiplicative and additive effects on the

spectra. The range of TSS, pH and firmness were 18.42 to 19.2 °Brix; 3.42 to 3.65 and 38.5 to 41.97 N, respectively.

### Analysis of spectral curves in reflectance and transmission modes

The typical raw reflectance and transmittance spectra from pomegranate fruit samples are shown in Fig. 2. This figure demonstrates the intensity differences between two spectral modes of reflectance and transmittance. As it can be seen from this figure, the most apparent difference between reflection and transmission is the spectral range. Reflected light could be detected across the range of spectrometer, while transmitted light was limited to a range of 600–950 nm because of low signal to noise ratio. Another distinction between spectral curves in two modes is the level of noise. Transmission spectra is noisier than reflectance spectra. Based on the previous studies such as Schaare and Fraser (2000), it can be related to the low amount of light penetrating into the fruit and it results in a reduced signal to noise ratio [34]. In order to overcome this difficulty, and to make accurate prediction models, preprocessing of spectra is essential. However, the spectra under reflectance and transmittance had similar characteristics. The absorbance in the range of 400–500 nm was due to the pigments. Right after the visible region, there

was a perceptible peak around 750 nm possibly because of the third overtone of O–H and the fourth overtone of C–H. Then in NIR region the transmittance had decreasing trend and a perceptible peak at around 970 nm because of the second overtone of O–H. Though, the spectral curves were rather flat for reflectance mode, the absorption peak around 970 nm could not be seen obviously. Considering the penetrating ability of VIS–NIR light and short integration time for reflectance, it was easy to understand why this happened: light could not carry much information of flesh in reflectance mode, which could be easily done for transmittance mode.

### PCA analysis

To obtain reference data for total soluble solid content, the cultivar was divided into three groups based on the limit values given in Table 1. PCA analysis performed after preliminary data treatment gave a classification probability of 96.4% at the 95% confidence level. The three groups can be clearly distinguished on Fig. 3, showing that classification on the basis of total soluble solids content correlates well with the recorded spectra. In this case, too, outliers which are the samples containing interferences with a negative influence on model development were removed. The PCA model was considered for five principal components, with an explained variance of 94%. Figure 3 shows the scatter plot of PCA score values in the first two PC spaces on the spectra preprocessed data for clustering of the pomegranate samples into the three groups. These two PCs summarize more variation in the data than any other pair of components. Therefore, this plot can be used to interpret differences and similarities among the samples.

### PLS calibration models of TSS, pH and firmness

Figures 4, 5, 6 show the scatter plots of the PLS predicted versus measured TSS, pH and firmness values. As can be seen, although the models based on two spectral modes could predict TSS, pH and firmness with high accuracy, reflectance mode made better prediction models in each case. As it was stated earlier, the reason can be attributed to the low amount of light penetrating into the flesh of the fruit which results in a reduced signal to noise ratio. The use of more intense light sources or a more sensitive spectrometer along with chemometrics can increase signal to noise levels and improve the transmission mode calibrations. In the following paragraphs, the developed PLS calibration models of both spectral modes for each three studied internal quality attributes of pomegranate are comprehensively discussed.

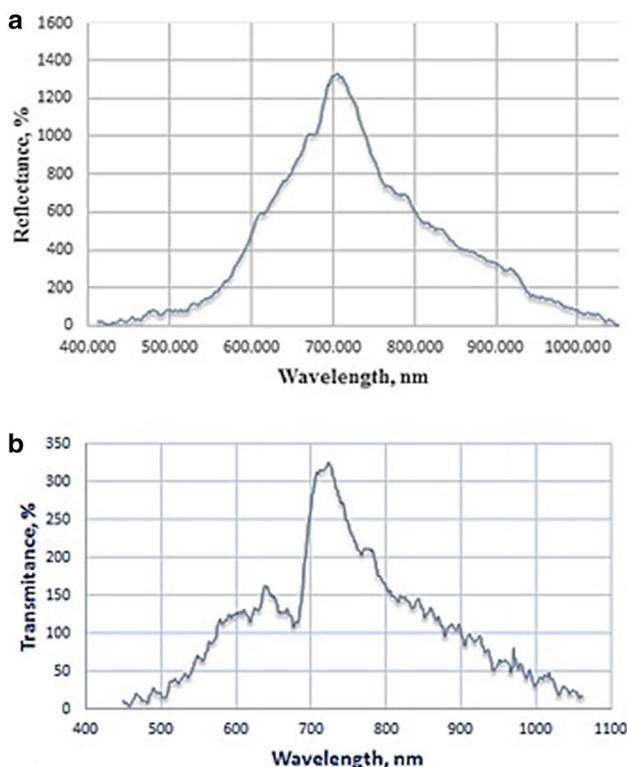
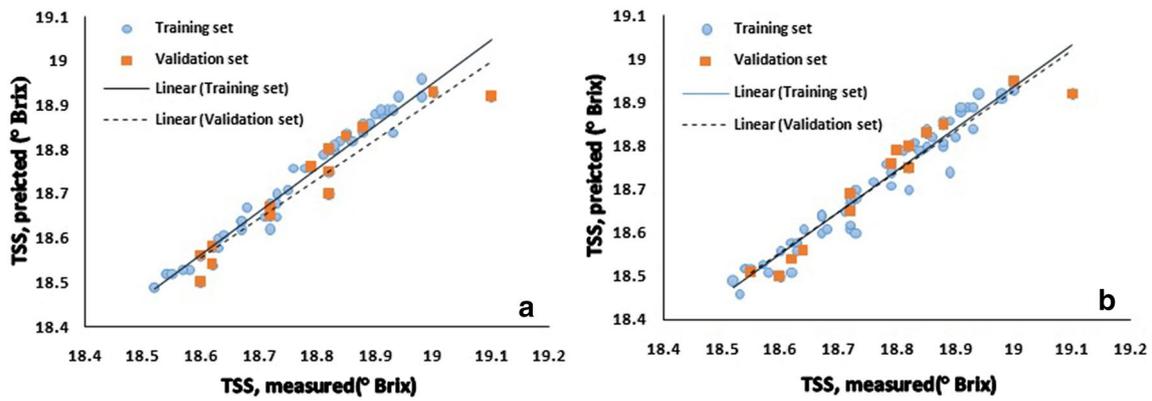
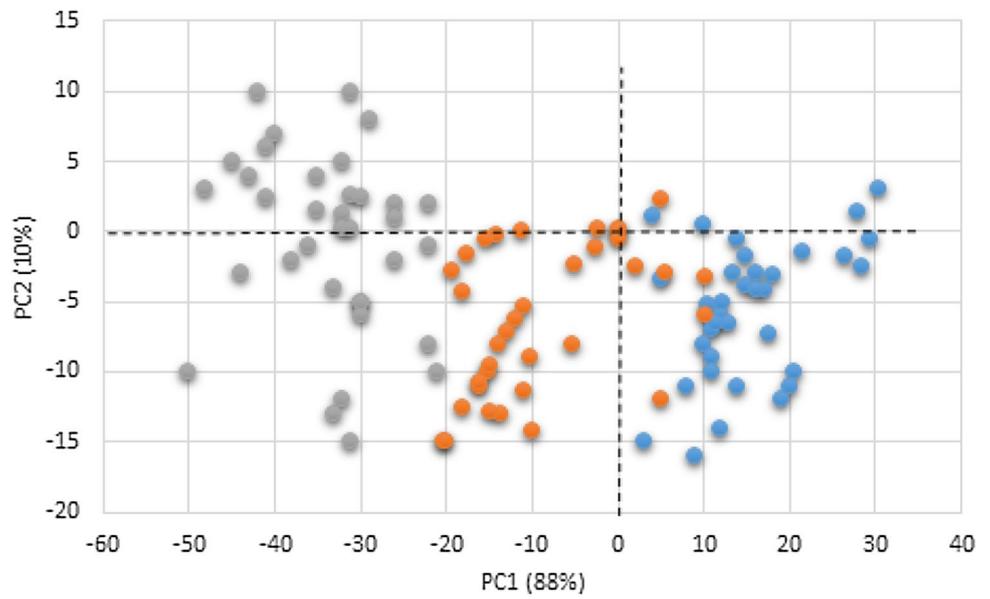
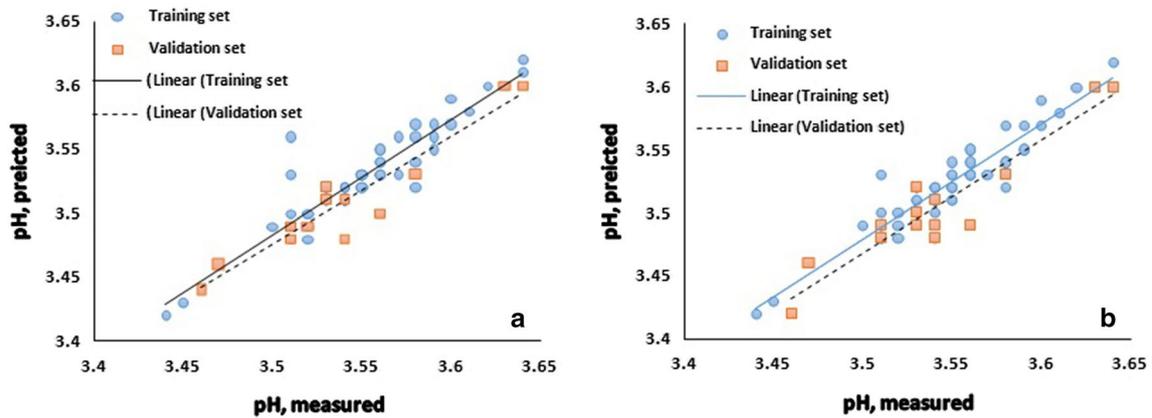


Fig. 2 Typical reflectance (a) and transmission (b) spectra

**Fig. 3** The scatter plots of PCA score values in the first two PC spaces for clustering of the pomegranates into the three classes



**Fig. 4** Comparison of predicted to measured pomegranate TSS for the reflectance (a) and transmittance (b) spectral modes



**Fig. 5** Comparison of predicted to measured pomegranate pH for the reflectance (a) and transmittance (b) spectral modes

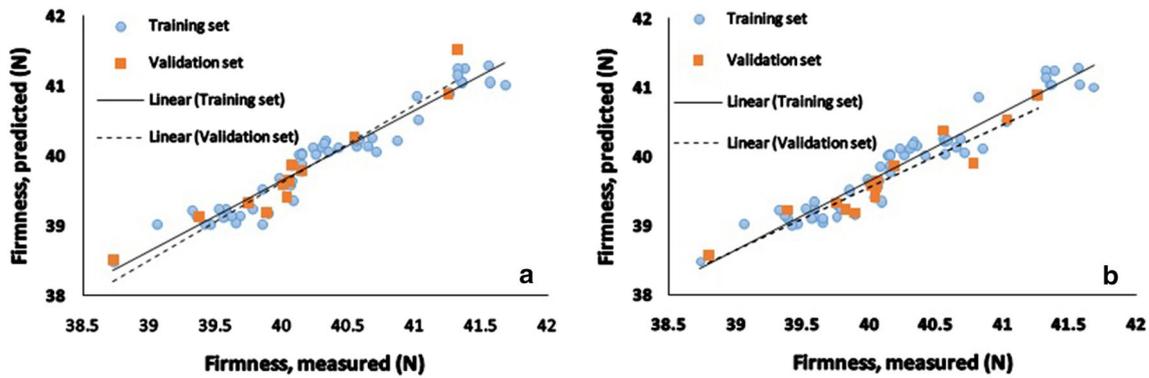


Fig. 6 Predicted versus measured pomegranate firmness in reflectance mode (a); transmittance mode (b)

### Total soluble solids (TSS)

As it is clear in Figs. 4, 5, 6, the PLS models could predict TSS better than the other studied quality parameters. This is in line with the findings that some researchers reported in prediction of samples taste attributes by NIR spectroscopy and PLS models. Their results showed that the PLS models could have better accuracy in prediction of TSS than of other taste characteristics for some vegetables and fruits such as cherry, tomato, and orange fruit [8, 23, 44]. Also the results of preprocessing of both spectral modes demonstrate that the PLS model with combination of SNV normalization, median filter smoothing and first derivative for preprocessing can yield better prediction of TSS. The reflectance mode can predict TSS with  $r=0.95$ ,  $RMSEC=0.22$  °Brix and  $RPD=6.7$  °Brix (Table 2). These parameters for the validation models were found to be:  $r=0.94$ ,  $RMSEP=0.21$  °Brix and  $RPD=6.72$  °Brix. In transmittance mode, the TSS was predicted with  $r=0.93$ ,  $RMSEC=0.22$  and  $RPD=6.4$  for the training set and  $r=0.92$ ,  $RMSEP=0.23$  and  $RPD=6.38$  resulted from the validation set (Table 3). To our knowledge, this is the first reported prediction of TSS in the literatures for pomegranate fruit from spectral data. Figure 4 shows the scatter plot presenting a linear correlation between the measured and predicted values of TSS from the best model. The best prediction statistics of TSS from calibration models for pomegranate fruit were reported  $R^2=78.1$ ,  $RPD=2.17$  by Arendse et al. (2018) [45].

### pH

The results of preprocessing of spectra for both modes show that the normalization, smoothing and transformation methods positively influenced the results of PLS models for pH prediction as SNV was slightly better than MSC when combined with each smoothing and transformation technique. For pH prediction, a PLS model preprocessed with the combination of SNV, median filter and second derivative

was found to be the best with  $r=0.85$ ,  $RMSEC=0.068$  °Brix and  $RPD=4.58$  °Brix for calibration set and  $r=0.86$ ,  $RMSEP=0.069$  °Brix and  $RPD=4.43$  °Brix for validation set (Table 2). The pH was predicted with  $r=0.83$ ,  $RMSEC=0.073$  and  $RPD=4.42$  for the training set and  $r=0.81$ ,  $RMSEP=0.072$  and  $RPD=4.39$  resulted from the validation sets by transmittance mode (Table 3). Figure 5 shows the scatter plot of correlation between the measured and predicted values of pH for the best model. As it can be seen, the prediction result of pH was not as accurate as the results of TSS prediction. However, the  $RMSEC$  and  $RMSEP$  of pH prediction in this research were found to be less. As stated earlier, there is no published results available on the NIR spectroscopy of pomegranate fruit and its arils. However, Zhang and McCarthy developed a PLS model to predict pomegranate pH from NMR data with  $r=0.77$  and  $RMSECV=0.13$  [46]. They reported that the  $RMSECV$  was very low and close to  $RMSEC$ , which means the loss in the accuracy was very when the calibration models were applied to the test data.

### Firmness

Similar to the models for predicting pomegranates pH and TSS, the SNV method was preferable against MSC normalizing method to develop the PLS model for predicting pomegranates firmness too. The best model for the prediction of firmness was achieved when SNV, median filter and first derivative were used as pre-processing, which was similar to what was found to be the best preprocessing for prediction of TSS too. The scatter plot of the correlation between measured and predicted values of firmness using the best selected model for both spectral modes is shown in Fig. 6. Results indicated that Vis/NIR spectroscopy had the potential to predict firmness directly and as accurate as it predicts TSS. The obtained statistical parameters for the best model in reflectance mode were:  $r=0.94$ ,  $RMSEC=0.65$  and  $RPD=5.65$  for calibration set and  $r=0.94$ ,  $RMSEP=0.68$

**Table 2** The results of calibration and prediction of PLS models with preprocessing techniques for reflectance mode

Preprocessing	Features	PCs	Calibration set			Prediction set		
			r	RPD	RMSEC	r	RPD	RMSEP
Original data	pH	15	0.66	2.01	0.332	0.67	1.97	0.245
	TSS	15	0.71	2.19	0.76	0.73	2.26	0.72
	Firmness	15	0.68	2.05	0.73	0.65	2.02	0.69
SNV, Median filter, D <sup>1</sup>	pH	9	0.84	4.41	0.073	0.85	4.37	0.071
	TSS	9	0.93	6.4	0.22	0.92	6.38	0.23
	Firmness	9	0.88	5.25	0.20	0.89	5.38	0.22
SNV, Savitzkye Golay, D <sup>1</sup>	pH	8	0.79	4.01	0.076	0.8	3.96	0.078
	TSS	8	0.88	4.95	0.37	0.88	5.01	0.38
	Firmness	8	0.80	4.76	0.32	0.79	4.89	0.35
SNV, Median filter, D <sup>1</sup> and mean center	pH	8	0.82	4.76	0.071	0.81	4.73	0.068
	TSS	8	0.95	6.7	0.22	0.94	6.72	0.21
	Firmness	8	0.94	5.65	0.65	0.94	5.33	0.68
SNV, Median filter, D <sup>2</sup> and mean center	pH	9	0.85	4.58	0.068	0.86	4.43	0.069
	TSS	9	0.87	4.32	0.29	0.87	4.28	0.29
	Firmness	9	0.88	4.75	0.24	0.89	4.63	0.25
MSC, Median filter, D <sup>1</sup>	pH	8	0.81	3.22	0.073	0.82	3.16	0.075
	TSS	8	0.9	4.15	0.34	0.9	4.09	0.35
	Firmness	8	0.89	4.45	0.53	0.9	4.56	0.52
MSC, Savitzkye Golay, D <sup>1</sup>	pH	9	0.79	3.13	0.135	0.8	3.12	0.136
	TSS	9	0.86	4.11	0.51	0.88	4.06	0.5
	Firmness	9	0.85	4.71	0.75	0.86	4.70	0.72
MSC, Median filter, D <sup>1</sup> and mean center	pH	8	0.82	3.35	0.098	0.81	3.15	0.082
	TSS	8	0.89	3.88	0.38	0.89	3.79	0.39
	Firmness	8	0.85	4.15	0.62	0.84	4.09	0.63
MSC, Median filter, D <sup>2</sup> and mean center	pH	8	0.81	2.85	0.134	0.82	3.03	0.115
	TSS	8	0.84	3.43	0.42	0.87	3.39	0.43
	Firmness	8	0.88	3.95	0.38	0.89	3.859	0.41

and RPD = 5.33 for prediction set (Table 2). These parameters for calibration model in transmittance mode were  $r = 0.91$ , RMSEC = 0.72 and RPD = 5.25. Also, these values for validation set of transmittance mode were  $r = 0.9$ , RMSEC = 0.73 and RPD = 5.12 (Table 3). The best prediction statistics of firmness from calibration models for pomegranate fruit were reported  $R^2 = 83.0$ , RPD = 2.43 by Arendse et al. (2018) [46].

### Comparing predicting results of PLS models in two spectral modes

In the present study, two spectral modes (reflectance and transmittance) were applied to acquire spectra of samples, and the comparison of the two modes was conducted in terms of different wavelength regions and PLS calibration models. As discussed earlier, spectra from reflectance mode in VIS–NIR region could provide as the best inputs to the PLS model used in prediction of pomegranates quality attributes. The reason may be attributed to the low amount of light penetrating in fruit which results in a reduced signal

to noise ratio. This result was in agreement with the findings by Cayuela and Weiland [47]. These researchers also recommended spectra in reflectance mode, considering that the measurements in transmittance mode were likely to be more influenced by fruit size, the amount of light penetrating fruit often being very small, making it difficult to acquire accurate transmittance measurements at grading line speeds. However, there have been some other researchers such as Schaare and Fraser; Fu et al.; Xing and Guyer; Wang et al.; Wang et al. who reported a little higher predictive outcomes using transmittance mode in contrast with reflectance [11, 33–36].

### Conclusion

This study compared the relative accuracy of reflectance and transmission modes of NIR spectroscopy for estimating TSS, pH and firmness of pomegranate fruit, and evaluated the optimal method for deriving the calibration. Good calibrations were obtained in each mode, supporting the use of NIR spectroscopy for the rapid and non-destructive

**Table 3** The results of calibration and prediction of PLS models with preprocessing techniques for transmittance mode

Preprocessing	Features	PCs	Calibration set			Prediction set		
			r	RPD	RMSEC	r	RPD	RMSEP
Original data	pH	15	0.64	1.95	0.586	0.62	1.91	0.486
	TSS	15	0.7	2.01	0.79	0.69	2.03	0.72
	Firmness	15	0.65	2.02	0.83	0.63	2.05	0.81
SNV, Median filter, D <sup>1</sup>	pH	9	0.82	4.33	0.079	0.8	4.21	0.076
	TSS	9	0.91	6.25	0.28	0.9	6.23	0.25
	Firmness	9	0.85	5.05	0.22	0.81	5.01	0.20
SNV, Savitzkye Golay, D <sup>1</sup>	pH	8	0.76	3.86	0.079	0.74	3.52	0.072
	TSS	8	0.84	4.85	0.47	0.81	4.28	0.44
	Firmness	8	0.80	4.52	0.38	0.78	4.42	0.36
SNV, Median filter, D <sup>1</sup> and mean center	pH	8	0.79	4.48	0.07	0.78	4.43	0.06
	TSS	8	0.93	6.4	0.22	0.92	6.38	0.23
	Firmness	8	0.91	5.25	0.72	0.9	5.12	0.73
SNV, Median filter, D <sup>2</sup> and mean center	pH	9	0.83	4.42	0.073	0.81	4.39	0.072
	TSS	9	0.82	4.24	0.35	0.8	4.04	0.31
	Firmness	9	0.81	4.45	0.29	0.81	4.15	0.22
MSC, Median filter, D <sup>1</sup>	pH	8	0.8	3.11	0.079	0.76	3.03	0.071
	TSS	8	0.88	4.03	0.42	0.83	4.01	0.42
	Firmness	8	0.85	4.26	0.55	0.81	4.15	0.54
MSC, Savitzkye Golay, D <sup>1</sup>	pH	9	0.74	3.05	0.225	0.72	3.01	0.223
	TSS	9	0.82	3.86	0.58	0.81	3.75	0.55
	Firmness	9	0.81	4.53	0.85	0.8	4.42	0.84
MSC, Median filter, D <sup>1</sup> and mean center	pH	8	0.8	3.16	0.099	0.76	3.05	0.096
	TSS	8	0.83	3.54	0.33	0.81	3.14	0.38
	Firmness	8	0.82	4.02	0.6	0.8	4.01	0.62
MSC, Median filter, D <sup>2</sup> and mean center	pH	8	0.8	2.68	0.225	0.76	2.28	0.223
	TSS	8	0.81	3.23	0.48	0.78	3.11	0.47
	Firmness	8	0.83	3.76	0.43	0.81	3.745	0.41

evaluation of pomegranate internal qualities. The results showed that the reflectance mode was more suitable than transmittance mode in the assessment of internal quality attributes for pomegranate fruit. The reason may be related to the size of pomegranate fruit that influences the transmittance signal more than the reflectance signal. PLS proved to be the most robust algorithm of those tested for generating calibration models. However, further research needs to be done to study and to understand the reasoning behind the effect of size on the transmittance spectra.

**Acknowledgements** The authors would like to thank Ferdowsi University of Mashhad for providing the laboratory facilities and financial support through the project No. of 28580.

## References

- O.A. Fawole, U.L. Opara, Developmental changes in maturity indices of pomegranate fruit: a descriptive review. *Sci. Hortic.* **159**, 152–161 (2013)
- O.A. Fawole, U.L. Opara, Changes in physical properties, chemical and elemental composition and antioxidant capacity of pomegranate (cv. ‘Ruby’) fruit at five maturity stages. *Sci. Hortic.* **150**, 37–46 (2013)
- O.A. Fawole, U.L. Opara, Fruit growth dynamics, respiration rate and physico-textural properties during pomegranate development and ripening. *Sci. Hortic.* **157**, 90–98 (2013)
- B.P. Khatiwada, P.P. Subedi, C. Hayes, L.C. Cunha Carlos Jr., K.B. Walsh, Assessment of internal flesh browning in intact apple using visible-short wave near infrared spectroscopy. *Postharvest. Biol. Technol.* **120**, 103–111 (2016)
- S. Bureau, D. Ruiz, M. Reich, B. Gouble, D. Bertrand, J.M. Audergon, C. Renard, Rapid and non-destructive analysis of apricot fruit quality using FT-near-infrared spectroscopy. *Food. Chem.* **113**, 1323–1328 (2009)
- C.J. Clark, V.A. McGlone, R.B. Jordan, Detection of brownheart in braeburn apple by transmission NIR spectroscopy. *Postharvest. Biol. Technol.* **28**, 87–96 (2003)
- J. Tarkosova, J. Copikova, Determination of carbohydrate content in bananas during ripening and storage by near infrared spectroscopy. *J. Near. Infrared. Spectrosc.* **8**, 21–26 (2000)
- R. Lu, Predicting firmness and sugar content of sweet cherries using near-infrared diffuse reflectance spectroscopy. *Trans. ASAE* **44**, 1265–1271 (2001)
- Y. Zhang, W.S. Lee, M. Li, L. Zheng, M.A. Ritenour, Non-destructive recognition and classification of citrus fruit

- blemishes based on ant colony optimized spectral information. *Postharvest. Biol. Technol.* **143**, 119–128 (2018)
10. H. Xiao, A. Li, M. Li, Y. Sun, K. Tu, S. Wang, L. Pan, Quality assessment and discrimination of intact white and red grapes from *Vitis vinifera* L. at five ripening stages by visible and near-infrared spectroscopy. *Sci. Hortic.* **233**, 99–107 (2018)
  11. J. Wang, K. Nakano, S. Ohashi, K. Takizawa, J.G. He, Comparison of different modes of visible and near-infrared spectroscopy for detecting internal insect infestation in jujubes. *J. Food. Eng.* **101**(1), 78–84 (2010)
  12. A. Moghimi, M.H. Aghkhani, A. Sazgarnia, M. Sarmad, Vis/NIR spectroscopy and chemometrics for the prediction of soluble solids content and acidity (pH) of kiwifruit. *Biosyst. Eng.* **106**, 295–302 (2010)
  13. Y.D. Liu, X.D. Sun, A.G. Ouyang, Nondestructive measurement of soluble solid content of navel orange fruit by visible-NIR spectrometric technique with PLSR and PCA-BPNN. *LWT-Food Sci. Technol.* **43**, 602–607 (2010)
  14. S. Saranwong, J. Sornsrivichai, S. Kawano, Prediction of ripe-stage eating quality of mango fruit from its harvest quality measured nondestructively by near-infrared spectroscopy. *Postharvest. Biol. Technol.* **31**, 137–145 (2004)
  15. W. Guo, J. Gu, D. Liu, L. Shang, Peach variety identification using near-infrared diffuse reflectance spectroscopy. *Comput. Electron. Agric.* **123**, 297–303 (2016)
  16. X. Tian, Q. Wang, J. Li, F. Peng, W. Huang, Non-destructive prediction of soluble solids content of pear based on fruit surface feature classification and multivariate regression analysis. *Infrared Phys. Technol.* **92**, 336–344 (2018)
  17. H. Schulz, M. Baranska, R. Quilitzsch, W. Schutze, G. Losing, Characterization of peppercorn, pepper oil, and pepper oleoresin by vibrational spectroscopy methods. *J. Agric. Food Chem.* **53**, 3358–3363 (2005)
  18. M. Golic, K.B. Walsh, Robustness of calibration models based on near infrared spectroscopy for the in-line grading of stone fruit for total soluble solids content. *Anal. Chim. Acta* **555**, 286–291 (2006)
  19. K.S. Chia, H. Abdul Rahim, R. Abdul Rahim, Prediction of soluble solids content of pineapple via non-invasive low cost visible and shortwave near infrared spectroscopy and artificial neural network. *Biosyst. Eng.* **113**, 158–165 (2012)
  20. E. Arendse, O.A. Fawole, L.S. Magwaza, H.H. Nieuwoudt, U.L. Opara, Development of calibration models for the evaluation of pomegranate aril quality by Fourier-transform near infrared spectroscopy combined with chemometrics. *Biosyst. Eng.* **159**, 22–32 (2017)
  21. B. Jamshidi, E. Mohajerani, H. Farazmand, A. Mahmoudi, A. Hemmati, Pattern recognition-based optical technique for non-destructive detection of *Ectomyelois ceratoniae* infestation in pomegranates during hidden activity of the larvae. *Spectrochim. Acta. Part A* **206**, 552–557 (2019)
  22. R.L. Long, K.B. Walsh, Limitations to the measurement of intact melon total soluble solids using near infrared spectroscopy. *Aust. J. Agric. Res.* **57**, 403–410 (2006)
  23. Y. Huang, R. Lu, K. Chen, Prediction of firmness parameters of tomatoes by portable visible and near-infrared spectroscopy. *J. Food. Eng.* **222**, 185–198 (2017)
  24. B.M. Nicolai, K. Beullens, E. Bobelyn, A. Peirs, W. Saeys, K.I. Theron, J. Lammertyn, Nondestructive measurement of fruit and vegetable quality by means of NIR spectroscopy: a review. *Postharvest. Biol. Technol.* **46**, 99–118 (2007)
  25. Y.H. Shao, Y. He, Y.D. Bao, J.Y. Mao, Near-infrared spectroscopy for classification of oranges and prediction of the sugar content. *Int. J. Food Prop.* **12**, 644–658 (2009)
  26. E.D. Louw, K.I. Theron, Robust prediction models for quality parameters in Japanese plums (*Prunus salicina* L.) using NIR spectroscopy. *Postharvest. Biol. Technol.* **58**, 176–184 (2010)
  27. C.Y. Liew, C.Y. Lau, Determination of quality parameters in Cavendish banana during ripening by NIR spectroscopy. *Int. Food Res. J.* **19**, 751–758 (2012)
  28. J. Li, W. Huang, C. Zhao, B. Zhang, A comparative study for the quantitative determination of soluble solids content, pH and firmness of pears by Vis/NIR spectroscopy. *J. Food. Eng.* **116**(2), 324–332 (2013)
  29. P.R. Armstrong, Rapid single-kernel NIR measurement of grain and oil-seed attributes. *Appl. Eng. Agric.* **22**(5), 767–772 (2006)
  30. S. Teerachaichayut, K.Y. Kil, A. Terdwongworakul, W. Thanapase, Y. Nakanishi, Non-destructive prediction of translucent flesh disorder in intact mangosteen by short wavelength near infrared spectroscopy. *Postharvest. Biol. Technol.* **43**, 202–206 (2007)
  31. Y. Liu, Y. Ying, Use of FT-NIR spectrometry in non-invasive measurements of internal quality of ‘Fuji’ apples. *Postharvest. Biol. Technol.* **37**, 65–71 (2005)
  32. P. Sirisomboon, M. Tanaka, S. Fujita, T. Kojima, Evaluation of pectin constituents of Japanese pear by near infrared spectroscopy. *J. Food. Eng.* **78**, 701–707 (2007)
  33. A. Wang, D. Hu, L. Xie, 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. *J. Food. Eng.* **126**, 126–132 (2014)
  34. P.N. Schaare, D.G. Fraser, Comparison of reflectance, intertance and transmission modes of visible-near infrared spectroscopy for measuring internal properties of kiwifruit (*Actinidia chinensis*). *Postharvest. Biol. Technol.* **20**, 175–184 (2000)
  35. X. Fu, Y. Ying, H. Lu, H. Xu, Comparison of diffuse reflectance and transmission mode of visible-near infrared spectroscopy for detecting brown heart of pear. *J. Food. Eng.* **83**(3), 317–323 (2007)
  36. J. Xing, D. Guyer, Comparison of transmittance and reflectance to detect insect infestation in Montmorency tart cherry. *Comput. Electron. Agric.* **64**(2), 194–201 (2008)
  37. N.N. Mohsenin, *Physical Properties of Plant and Animal Materials. 2nd Revised and Updated Edition* (Gordon and Breach Science Publishers, New York, 1986)
  38. H. Cen, Y. He, Theory and application of near infrared reflectance spectroscopy in determination of food quality. *Trends Food Sci. Technol.* **18**, 72–83 (2007)
  39. T. Næs, T. Isaksson, T. Fearn, T. Davies, *A User-friendly Guide to Multivariate Calibration and Classification* (NIR Publications, Charlton, 2004)
  40. M.L. Vigni, C. Durante, M. Cocchi, Exploratory data analysis, in *Chemometrics in Food Chemistry*, ed. by F. Marini (Elsevier, Amsterdam, 2013), pp. 55–126
  41. R.A. Viscarra Rossel, ParLeS: software for chemometric analysis of spectroscopic data. *Chemom. Intell. Lab. Syst.* **90**, 72–83 (2008)
  42. Y. Liu, X. Sun, A. Ouyang, Nondestructive measurement of soluble solids content of navel orange fruit by visible-NIR spectrometric technique with PLSR and PCA-BPNN. *LWT-Food Sci. Technol.* **43**, 602–607 (2010)
  43. F. Westad, M. Bevilacqua, F. Marini, Regression, in *Chemometrics in Food Chemistry*, ed. by F. Marini (Elsevier, Amsterdam, 2013), pp. 127–169
  44. B. Jamshidi, S. Minaei, E. Mohajerani, H. Ghassemian, Reflectance Vis/NIR spectroscopy for nondestructive taste characterization of Valencia oranges. *Comput. Electron. Agric.* **85**, 64–69 (2012)
  45. E. Arendse, O.A. Fawole, L.S. Magwaza, L.H. Nieuwoudt, U.L. Opara, Fourier transform near infrared diffuse reflectance

spectroscopy and two spectral acquisition modes for evaluation of external and internal quality of intact pomegranate fruit. *Postharvest. Biol. Technol.* **138**, 91–98 (2018)

46. L. Zhang, M.J. McCarthy, Assessment of pomegranate postharvest quality using nuclear magnetic resonance. *Postharvest. Biol. Technol.* **77**, 59–66 (2013)
47. J.A. Cayuela, C. Weiland, Intact orange quality prediction with two portable NIR spectrometers. *Postharvest. Biol. Technol.* **58**, 113–120 (2010)

**Publisher's Note** Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.