Non-Destructive Quality Measurement for Three Varieties of Tomato Using VIS/NIR Spectroscopy

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Abstract: The non-destructive visible/near-infrared (VIS/NIR) spectroscopy is a promising technique in determining the quality of agricultural commodities. Therefore, this study aimed to examine the ability of VIS/NIR spectroscopy (550–1100 nm) to distinguish between three different varieties of tomato (i.e., Ekram, Harver and Izmer), as well as to predict the quality parameters of tomato, such as soluble solids content (SSC), titratable acidity (TA), taste (SSC/TA) and firmness. Ninety intact samples from three tomato varieties were used. These samples were examined using VIS/NIR spectroscopy and quality parameters were also measured using traditional methods. Principal component analysis (PCA) and partial least square (PLS) were carried out. The results of PCA showed the ability of VIS/NIR spectroscopy to distinguish between the three varieties, where two PCs explained about 99% of the total variance in both calibration and validation sets. Moreover, PLS showed the possibility of modelling quality parameters. The correlation coefficient ($R^2$) and the ratio of performance deviation (RPD) for all quality parameters (except for firmness) were found to be higher than 0.85 and 2.5, respectively. Thus, these results indicate that the VIS/NIR spectroscopy can be used to discriminate between different varieties of tomato and predict their quality parameters.

Keywords: VIS/NIR spectroscopy; tomato varieties; tomato quality; principal component analysis (PCA); partial least squares (PLS)

1. Introduction

Tomato (Solanum lycopersicum E.) is considered one of the most important food crops in the world, where global consumption is estimated at 6.4 million tons per year for both fresh and industry [1,2]. Tomato has many nutritional benefits, such as it contains vitamins C, A and K [3].

The three most important tomato varieties grown in Palestine are Ekram, Izmer and Harver, where the Ekram variety is distinguished by its high production, long shelf life, very firm fruit and good low-temperature setting. Whereas, the Izmer variety has consistent fruit size and shape, very good heat tolerance and setting ability under hot conditions. Finally, the Harver variety is considered one of the most cultivated varieties, characterized by a homogeneous size and suitable for moderate to hot conditions [4].

In recent years, there has been considerable interest in the quality of fruits by the consumer and food industry [5,6]. Soluble solids content (SSC), titratable acidity (TA), taste and firmness are the primary quality characteristics of tomato fruit, which directly affect consumer acceptance and the industries standard. Taste is composed of sweetness and acidity and can be expressed by SSC to TA ratio [7–9]. Tomato fruits high in both sugar and acidity content have good taste. While the high acidity and low sugar content will give a bland tomato taste, if the sugar content is high and the acidity content is low, it will give a tasteless tomato [10,11].

Different types of tomato have SSC, TA, taste and firmness/hardness. This affects the opinion of the consumer and also on the product, so it is important to distinguish between the different tomato varieties [12].
These quality parameters of tomato are usually evaluated using traditional methods, which are destructive, time-consuming and costly [13,14]. Thus, there is a need for non-destructive, fast and environmentally friendly methods to monitor the quality of fruits and to determine the appropriate time for harvesting to provide losses and maximize income [15,16].

One of these methods is visible/near-infrared (VIS/NIR) spectroscopy [17,18]. The principle of the VIS/NIR technique is based on the absorption of energy by the functional groups (e.g., R-OH, R-CH, O-H and C-H) present in the fruits, which causes vibration of molecules, and this forms acquired spectra [19]. The VIS/NIR technology can be applied in many ways, i.e., reflectance, transmittance and interactance mode. However, the best way to obtain internal information from the fruit is the reflectance mode [20].

The extraction of useful information from spectra data depends on multivariate data analysis (MVDA) methods, such as principal component analysis (PCA), which is applied initially to distinguish between samples [21–23]. Additionally, partial least squares (PLS) can be applied as a prediction method. It is based on the link between two matrices x and y, one of them is taken from spectra data and the other is a reference [24,25]. After building a PLS model, there are important parameters that are used to evaluate the strength of the prediction model, such as correlation coefficient ($R^2$), the root mean squared error (RMSE) and the ratio of performance deviation (RPD) [26,27]. Where a good model should have, e.g., a higher $R^2$ (close to 1), lower RMSE, RPD value greater than 2 and small differences between the results of calibration and validation sets [28].

The VIS/NIR spectroscopy has been widely applied to measure the external and internal properties of fruits such as tomato [29,30] and pear [31]. Beghi et al. [32] tested the ability of VIS/NIR spectroscopy (450–2500 nm) to predict the SSC of tomato fruit. The authors were able to build a PLS model with $R^2$ 0.8 and RPD 2.5. Moreover, Li et al. [33] used VIS/NIR spectroscopy (550–1100 nm) to distinguish between three varieties of melon based on SSC. They have built a PCA model with two PCs that explained 95% of the total variance and a PLS model with $R^2$ of 0.8 and RMSE of 0.7, their results showed the ability of VIS/NIR spectroscopy to predict the SSC parameter for different varieties of melon. In addition, VIS/NIR spectroscopy was used to predict fruit taste (SSC/TA) such as tomato, apple and orange in several studies [9,34].

To our best knowledge, there are no previous studies to investigate the quality of these varieties (i.e., Izmer, Ekram and Harver) used in our study. Therefore, this study was aimed to use VIS/NIR technique with a range of 550–1100 nm to distinguish between three tomato varieties (i.e., Ekram, Harver and Izmer) and to build a relationship between the spectra acquired from the VIS/NIR spectroscopy and quality parameters (i.e., SSC, TA, taste (SSC/TA) and firmness) for the three tomato varieties.

2. Materials and Methods

2.1. Tomato Samples Collecting

A total of 90 tomato samples (30 samples for each variety) and ripening stages light red according to the United States Standards for Grades of Fresh Tomatoes [30] were used for this study. The samples were collected from a farm near Tulkarm, Palestine in October 2019 and were grown inside greenhouses under the same conditions. The fruits were stored at room temperature of 25 ± 1 °C for one day before starting the examinations to ensure the samples reach an equilibrium temperature with the laboratory environment. The VIS/NIR measurement and quality reference were carried out the next day [35,36].

2.2. Spectral Measurements

The VIS/NIR spectroscopy with a USB 2000+ miniature fiber optic spectrometer (Ocean Optics, Orlando, FL, USA). Vivo light source with a 50 μm fiber optics probe was used to obtain spectra in reflectance mode (R) and, then, recorded as absorbance (i.e., log (1/R)). The spectra range was 550–1100 nm, and the integration time was 360 μs. Three reflection spectra (550–1100 nm) were taken in three positions at equal distances around
the equator (about 120°) for each tomato after placing it on the light source. Each sample was measured three times and later the average was taken. Additionally, the reference standard was applied every 10 min [37].

2.3. Data Collected
Spectra data were collected for later analysis using the Unscrambler program (version 10.3, Camo Software AS, Oslo, Norway).

2.4. Quality Parameters Test
The quality parameters of each variety were measured. Firmness was measured using a manual fruit penetrometer (Total, model GY-4, Beijing, China), and the examination was repeated three times for each sample; the results are expressed in Newton units (N) (Feng et al. 2019). After that, tomato juice samples were extracted to evaluate SSC and TA that were measured using a portable device (Atago, Cat. No. 39005 Pal-Bx/Acid F5, Bellevue, WA, USA). SSC was measured first and, then, TA by the same device. Distilled water (DW) was used to dilute the tomato juice according to 0.04% citric acid standard reference, where 1.0 mL of tomato juice was added and diluted with 49.0 mL with DW. SSC and TA were measured in triplicate, and the results were expressed in Brix and percentage (%), respectively. The taste (which is dimensionless) was calculated according to the following Equation (1) [11]:

\[
\text{Taste} = \frac{\text{SSC}}{\text{TA}}
\]  

2.5. Statistical Analysis
Statistical analysis was applied to prove differences in quality parameters (SSC, TA, taste and firmness) between three varieties (Ekram, Harver and Izmer). One-way ANOVA was applied at a 5% significance level to identify the differences between the varieties using the Excel program (2013, Microsoft Office, Microsoft, Redmond, WA, USA) [38].

2.6. Spectra Pre-Processing
First derivatives (1st D) of the acquired spectra based on Savitzky–Golay (SG) were carried out to increase the spectral resolution [39,40].

2.7. Principal Component Analysis (PCA)
PCA with test set validation was carried out for the VIS/NIR region (550–1100 nm), where the tomato samples for three varieties (i.e., Ekram, Harver and Izmer) were divided into calibration set (60 samples) and validation set (30 samples), taking into consideration that the three varieties were represented in each set [41].

2.8. Partial Least Squares (PLS)
Then PLS-1 models for spectral data with SSC, TA, taste and firmness were applied separately for each variety, where full cross-validation was used (30 samples for each variety). Furthermore, models for each quality parameter were built for all the varieties together using 60 and 30 samples for the calibration and validation set, respectively [42].

2.9. Model Performance
The evaluation of PLS models was done according to the \( R^2 \), RPD, relative error (RE) and RMSE [18,43].

3. Results and Discussion
3.1. Statistical Analysis
Table 1 shows the statics of quality parameters, i.e., SSC, TA, taste and firmness of the three tomato varieties. There was a significant difference between the varieties at \( p \leq 0.05 \). These results seem to be similar to those results reached by Saad et al. [44]
for tomato quality parameters (such as SSC) and Machado et al. [31] who differentiated between three varieties of pear based on their quality characteristics (such as firmness).

Table 1. Descriptive statistical of quality parameters for three tomato varieties.

| Quality Parameters * | Tomato Varieties |
|----------------------|------------------|
|                      | Ekram            |
|                      | Harver           |
|                      | Izmer            |
| Mean (SD **)         | Max   | Min   | Range | Mean (SD **) | Max   | Min   | Range | Mean (SD **) | Max   | Min   | Range | p     |
| SSC (Brix°)          | 5.1 (0.4) | 5.9   | 4.3   | 5.1 (0.4) | 4.8   | 3     | 3.9   | 4.6 (0.5)   | 5.7   | 4     | 4.8   | <0.05 |
| TA (%)               | 1.3 (0.2) | 1.7   | 0.9   | 1.3 (0.4) | 0.6   | 0.1   | 0.3   | 0.4 (0.1)   | 0.6   | 0.1   | 0.3   | 0.05  |
| Taste (SSC/TA)       | 3.4 (0.7) | 5     | 2.8   | 3.9   | 11    | 3.7   | 21    | 6.5 (4.4)   | 22    | 5.5   | 13.7  | <0.04 |
| Firmness (N)         | 17.5 (2.7) | 23    | 12.6  | 17.8  | 13.6  | 1.3   | 16    | 11.5 (14.9) | 2.3   | 19    | 11    | 15    |

* Normally distributed. ** SD: standard deviation

3.2. Spectral Characterization

Figure 1 shows the representative spectrum for the three tomato varieties with the 1st D in the range 550–1100 nm. The results showed some absorbance peaks due to the vibration of O-H, C-H and N-H bonds, which are related to inner fruit compositions such as sugar and acid. The absorption in the VIS region was owing to the fruit pigments such as chlorophyll, β-carotene and lycopene. The highest bands in the VIS region (peaks at 580 and 607 nm) are because of the absorption of the chlorophyll, β-carotene and lycopene similar to the results described for melon by Dull [45] and orange by Jamshidi et al. [9]. Likewise, the highest bands (peaks at 700, 813, 964, 980, 990, 1068 and 1097 nm) were in the NIR region, which are due to the C-H, O-H and N-H bonds similar to that reported by Radzevicius et al. [5] for tomato quality tested using VIS/NIR spectroscopy. Cen and He [17] and Li et al. [33] published that the penetration depth of NIR in the fruit was greater in the 750–1000 nm range than for other ranges.

Figure 1. The effect of the first derivatives (1st D) on the spectra obtained from tomato varieties. Ekram (blue), Harver (red) and Izmer (green).
3.3. Principal Component Analysis (PCA)

The PCA results for both calibration and validation sets showed the ability of VIS/NIR spectroscopy with range 550–1100 nm to fully distinguish between the three varieties, as can be seen in Figure 2 for the calibration set. Two PCs for calibration and validation sets explained 99% and 100% of the total variance, respectively.

![PCA scores plot](image)

**Figure 2.** PCA scores plot for the calibration set (60 samples) based on VIS/NIR (550–1100 nm) spectra for tomato varieties. Two PCs explained 99% of the total variance.

3.4. Partial Least Squares (PLS)

The PLS-1 results of quality parameters (i.e., SSC, TA, taste and firmness) for each variety are summarized in Table 2.

**Table 2.** PLS-1 models' results with full cross-validation for each tomato variety for their SSC, TA, taste (SSC/TA) and firmness.

| Model Parameters | SSC          | TA          | Taste (SSC/TA) | Firmness |
|------------------|--------------|-------------|----------------|----------|
|                  | Ekram | Harver | Izmer | Ekram | Harver | Izmer | Ekram | Harver | Izmer | Ekram | Harver | Izmer |
| $R^2$             | 0.97  | 0.98   | 0.98   | 0.98  | 0.91   | 0.91  | 0.94  | 0.91   | 0.92  | 0.70  | 0.74   | 0.72  |
| Slope            | 0.98  | 0.99   | 0.98   | 0.88  | 0.99   | 0.95  | 1.01  | 1.00   | 0.96  | 0.96  | 1.06   | 1.07  |
| RMSE             | 0.12  | 0.14   | 0.18   | 0.09  | 0.05   | 0.06  | 0.2   | 1.1    | 1.3   | 2.0   | 0.7    | 1.6   |
| RE%              | 2     | 3      | 3      | 7     | 12     | 1     | 10    | 8      | 11    | 10    | 10     | 10    |
| RPD              | 3.4   | 3.2    | 3      | 2.7   | 3      | 2.8   | 3.2   | 3.3    | 3     | 1.5   | 2      | 1.9   |

Additionally, the results of both calibration and validation sets are summarized in Table 3. Results showed that the PLS-1 models could predict more than one tomato quality parameter for each variety and all varieties (i.e., SSC, TA and taste). Moreover, all PLS-1 models showed good performance.

3.5. Soluble Solids Content (SSC)

PLS-1 models for Ekram, Harver and Izmer varieties could predict SSC with RMSE about 0.2, $R^2$ 0.98 and RPDs were 3.4, 3.2 and 3 for Ekram, Harver and Izmer varieties, respectively. REs were less than 4%. These results are in agreement with those reported by Machado et al. [31] to predict the SSC of different pear varieties using VIS/NIR spectroscopy. Besides, the PLS model for both calibration and validation had high performance and was close to each other. Where RMSEs were about 0.3, $R^2$ for calibration and validations were 0.97 and 0.98, respectively. Additionally, the models had good RPDs at about 3.5. This is in
agreement with the results reported by Radzevicius et al. [5] for SSC prediction of tomato fruit using VIS/NIR spectroscopy.

Table 3. PLS-1 models’ results for the calibration (cal) and validation (val) sets for quality parameters for three tomato varieties.

| Model Parameters | SSC | TA | Taste (SSC/TA) | Firmness |
|------------------|-----|----|----------------|----------|
| $R^2_{cal}$      | 0.97| 0.90| 0.94           | 0.7      |
| Slope$^2_{cal}$  | 0.99| 0.95| 0.93           | 0.99     |
| RMSEC            | 0.18| 0.17| 1.0            | 0.6      |
| RE$^2_{cal}$ %   | 0   | 16  | 9              | 0        |
| RMSEC            | 3.7 | 3   | 4.1            | 1.7      |
| RPD$^2_{cal}$    | 1.04| 0.93| 1.06           | 1.05     |
| Slope$^2_{val}$  | 0.22| 0.89| 0.94           | 0.71     |
| RMSEV            | 4   | 3   | 1.5            | 0.7      |
| RE$^2_{val}$ %   | 3.4 | 2.8 | 3.9            | 1.6      |

RMSEC: root mean squares error of calibration. RMSEV: root mean squares error of validation.

3.6. Titratable Acidity (TA)

PLS-1 models could predict TA for Izmer, Harver and Ekram. All models were considered acceptable models because they have low RMSE and high RPD, where RPD for Harver was the highest with a value of 3 and the lowest RMSE. However, $R^2$ for all varieties was high at about 0.9. Moreover, the results obtained from the three varieties of both calibration and validation sets showed that the VIS/NIR spectroscopy was able to predict TA. The RPDs were about 3, which makes the models excellent as reported by Feng et al. [46]. Additionally, $R^2$ for the calibration and validation sets were 0.90 and 0.89, respectively. These results were better than those obtained by Saad et al. [44] for TA of tomato using reflectance VIS/NIR (299–1100 nm) using PLS (i.e., RMSE 4.08 and $R^2$ 0.7).

3.7. Taste (SSC/TA)

PLS-1 results obtained from each variety indicated that VIS/NIR spectroscopy could predict tomato taste (SSC/TA) directly as accurate as it predicts SSC and TA separately. The reason is that SSC/TA depends on SSC and TA, as well as their chemical bonds such as C-H and O-H groups. According to the equation, taste = SSC/TA, when TA (acidity) is low, SSC/TA becomes high [11]. This is what was obtained from the results of this study for full cross-validation (30 samples for test set validation for each variety) (Figure 3a–c), where the models have high RPDs and $R^2$ about 3 and 0.92, respectively. These results seem to be similar to those reported by Jamshidi et al. [9], who investigated VIS/NIR with a range of 400–1100 nm for Valencia orange taste. Furthermore, the VIS/NIR spectroscopy could predict the taste of tomato for all varieties together, Figure 4 shows the PLS-1 model obtained from the test set-validation (i.e., 20 samples × 3 varieties = 60 samples). The RPDs for calibration and validation sets were 4.1 and 3.9, respectively. Additionally, $R^2$ was about 0.95, which makes the models excellent models [41].
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(a) The test set validation for 30 samples of Ekram variety. E: Ekram. (b) The test set validation for 30 samples of Harver variety. H: Harver. (c) The test set validation for 30 samples of Izmer variety. I: Izmer.

**Figure 3.** PLS model for taste (SSC/TA), full cross-validation, (a–c), with 30 samples for each variety were used.
3.8. Firmness

Despite the fact that VIS/NIR spectroscopy was able to predict tomato firmness for the varieties, the models are considered to be a lower standard ($R^2$, RPD and RMSE) than the ones obtained from SSC, TA and taste. However, the PLS models for Ekram, Harver and Izmer showed acceptable performance according to $R^2$ with a value of about 0.7 and RPDs greater than 1.5. The results of this part are in agreement with those published by Machado et al. [31] that applied VIS/NIR (600–1100 nm) to evaluate the firmness for three different pear varieties. In addition, the PLS results obtained from calibration and validation sets indicated the ability of VIS/NIR with range 550–1100 nm to predict the firmness, where $R^2$ was about 0.7 and RPDs more than 1.5. This is in arrangement with previous research that used VIS/NIR to evaluate fruit firmness such as tomato and apple [7,46].

When the values of RPD and $R^2$ are higher than 1.5 and 0.5, respectively, the model is considered acceptable as described by Ncama et al. [19] and Beghi et al. [47] for fruit quality evaluation using the PLS model.

The models achieved from this study can be considered acceptable models, since they showed excellent performance, and there are few differences between the results of calibration and validation sets. Especially, the PLS models for taste (SSC/TA), which showed that the VIS/NIR can predict the taste of different tomato varieties. Therefore, VIS/NIR can be considered to be an equivalent and alternative technique to evaluate the quality parameters instead of the traditional method.
4. Conclusions

The results of the study showed that the VIS/NIR spectroscopy can be used to classify three varieties of tomato, as well as determine their quality parameters, such as SSC, TA, taste (SSC/TA) and firmness, with good accuracy. This may open the door for using VIS/NIR spectroscopy as a sensor that can be inserted in the sorting system in the packing house and also the possibility of using portable VIS/NIR spectroscopy, which can be applied directly in the field or the market for quality control. Additionally, it suggests the possibility of having a field sensor system that can be applied to determine the appropriate harvesting time according to SSC, TA or taste (SSC/TA).

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