Multivariate Approach to the Measurement of Tomato Maturity and Gustatory Attributes and Their Rapid Assessment by Vis–NIR Spectroscopy

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Standard methods for determining quality and maturity are time- and labor-consuming and generally measure individual criteria at a specific time, without considering relationships among quality parameters. To propose a rapid and nondestructive analysis method describing multidimensional quality variables, an experiment was undertaken with mature green to overripe tomato fruits found on the North American retail markets. Factor analysis was used to analyze results. Four factors were considered, representing 81% of total variance. The first one, tomato maturity stage (TMS), is related to color, lycopene content, firmness, titratable acidity (TA), pH, and soluble solids (SS). Nondestructive rapid assessment by vis–NIR spectroscopy can predict TMS (r² = 0.93). Factors 2 and 3 are both related to taste and should be considered simultaneously. Factor 2, called the gustatory index, is linked to electrical conductivity (EC), SS, TA, and pH. Factor 3, defined by SS, can be directly measured by a refractometer. Four categories of taste are proposed; the most desirable one ranks high both in soluble solids (above 4.5° Brix) and in gustatory index (above 0). It was not possible to measure the gustatory index by vis–NIR spectroscopy (r² = 0.17), but it can be estimated by EC, using a simple formula. The proposed limit between high and low gustatory index then corresponds to an EC of 5.4 mS/cm. Factor 4, variety, mostly discriminates the pink tomato type and field-grown samples from other varieties.

KEYWORDS: Color; firmness; lycopene; Lycopersicon esculentum; factor analysis; soluble solids; taste; titratable acid; tomato maturity stage

INTRODUCTION

Tomato (Lycopersicon esculentum Mill.) maturity is usually assessed by fruit firmness and color (1, 2). Changes in firmness are highly correlated with external appearance characteristics of tomato (3). Color, which has been related to firmness, has also a strong influence on the initial purchase decision by consumers, who generally relate fruit color to its gustatory quality (1). Color evolution during fruit ripening is mainly related to the breakdown of chlorophyll and the increase of carotenoids such as lycopene, which is responsible for the red color and constitutes 75–83% of the total pigment content at full ripeness, whereas β-carotene shows a less marked increase compared to lycopene with about 3–8.4% of the total carotenoids (4–6). Molyneux et al. (7) found a strong effect of cultivar on color readings. Field-grown tomato breeding lines also differ in terms of fruit color (8). The a*/b* ratio proved to be better than a* or the tomato color index (TCI) to distinguish varieties (9). Using color as a main variable describing physiological fruit maturity is of course possible (10). However, firmness is poorly correlated with a*/b* values (6). Robust models are difficult to build, due to the fact that color is strongly dependent on cultivar and agricultural conditions and because storage conditions may significantly alter color development (11).

Beyond color and firmness, the maturity parameter should also include nutritional and organoleptic attributes as they vary according to the harvesting fruit stage and postharvest conditions (12). These new parameters are now important for consumers looking for healthy and tasteful fruits. Soluble sugar content and its interaction with organic acids are highly related to flavor quality (1) and are adversely affected by early harvest or chilling (13, 14). In fact, Raffo et al. (6) observed that dry matter and soluble solids of tomato during ripening were linearly and positively correlated to the ripening stage, whereas proteins, fats, fiber, and ash did not vary significantly during ripening. With
regard to organic acids, they observed a decline of citric acid, whereas malic and oxalic acid did not change markedly during ripening.

Several standard laboratory tests exist that measure various aspects of fruit quality. The major drawback of these methods is the need to destroy fruits to get the quality attributes. Spectroscopy is an alternative for high-speed, nondestructive, and simultaneous measurement of quality criteria on line (15–17), which paves the way for more biology-based measurements of fruit condition. For example, spectroscopy has been successfully tested as a rapid and nondestructive means to measure maturity of apples to determine the optimal timing for harvest (18). For green harvested tomato, a multispectral approach was superior to the standard colorimeter readings (19) to distinguish mature fruits from those that have not reached their physiological maturity (20). Near-infrared spectroscopy (NIRS) has also been used for avocado maturity determination, which depends on oil and dry matter content. In that particular case, color is a poor descriptor of maturity (21, 22). Similarly, estimating mango maturity at the mature-green stage, prior to the climacteric rise, is a difficult task that has a significant impact on postharvest sensory quality. NIRS has been used to determine mango internal quality parameters such as soluble solids, dry matter, and starch with sufficient accuracy to allow proper maturity assessment, even on the tree (23–25).

The goal of this study was to investigate the feasibility of considering tomato postharvest quality evolution with a multidimensional approach to develop (1) a global and multivariate maturity chart, which may characterize fruit physiological stage (26). The Hunter colorimeter (Hunter Associates Laboratory, Reston, VA) was configured for Hunterlab’s L, a, and b scale with daylight (D65) and a 10° observer. The three color variables were used to compute the tomato color index (TCI); TCI = 2000(1/(a² + b²))1/2. This is a single-number criteria used to measure tomato color (26). The Hunter a value of fruits under study ranged from −5.9 to 25.3, whereas the TCI ranged from −15.7 to 65.0. Tomato pericarp firmness was measured with a mechanical probe (Bareiss HP, Hohenheim, Baden-Württemberg, Germany; (27)). The device measured local pericarp movement upon application of a constant 12.5 N force using a 0.25 cm² cylindrical flat-ended probe. Result was in relative units from 0 (maximum pericarp displacement) to 100 (very hard; no pericarp displacement). Soluble solids measurement near tomato surface was done with an Atago refractometer (ATC 1E, Tokyo, Japan). A drop of liquid was obtained after locally removing the cuticle and breaking peripheral pericarp cells with a Paster pipe. For whole tomato extract soluble solids measurement, a benchtop device was used (ABBCE Mark II, Reichert Analytical Instruments, Depew, NY). A pH-meter (Orion Research Inc., Beverly, MA) was used, with a spear-type probe (Cole Parmer Instruments) for near-surface measurements inserted at a depth of about 5 mm in the pericarp. A standard combination probe was used for whole tomato extract. Electrical conductivity (mS/cm) was measured using a specific probe (Orion Research Inc.). Titratable acidity was measured using 15 mL of the whole tomato extract, titrated to pH 8.1 using 0.1 N NaOH (one measurement per fruit). The following formula was used for calculation: Z = (V × N + Meq × 100) / Y, where Z = titratable acidity (as % citric acid), V = volume of NaOH used, N = normality of NaOH, Meq = weight of a milliequivalent of citric acid (0.064 g), and Y = volume of tomato extract used (15 mL).

Lycopene level was determined according to the reduced volumes of organic solvents method of Fish et al. (28). The upper phase (hexane) was sampled to obtain an absorbance reading at 503 nm using a Varian Cary 500 (Varian Inc., Palo Alto, CA). The following relation was then used for estimation of lycopene content: lycopene (mg/kg) = (A380 × 31.2)/(quantity of tissue used) (28). The result for each tomato was an average of one reading for each of two extracts on the same homogenate.

Spectroscopic measurements were made with the Varian Cary 500 equipped with an integration sphere (LabSphere Inc., North Sutton, NH). The whole tomato was placed in such a way that the incident tungsten halogen light beam touched a selected sampling area, prior to closing a stray-light protection cover. The selected wavelength range used was from 400 to 1500 nm, with an integration time of 0.3 s and a reading at every 2 nm, for a total of 551 reflectance readings per sample area. Once a day, before starting actual measurements, a 0 reflectance (light path blocked) and 100% reflectance (using a PTFE diffuse reflectance standard) calibration was done. The result for each tomato was an average of four equidistant readings on the same fruit.

Data Analysis. A factor analysis was performed on the Y-variable data set (physicochemical data) to determine if individual variables could be combined to define some underlying multivariate quality parameter. In factor analysis, linear combinations of the variables are successively computed to maximize overall variability (29) followed by an axis rotation to facilitate interpretation. The first factor explains the highest proportion of data set variability (eigenvalue), the second factor represents the second highest eigenvalue, and so on. Factors are new, independent variables (not correlated among themselves). A value (score) can be calculated for each tomato on each factor. SAS (SAS Institute Inc., Cary, NC) was used for computation. Factors having an eigenvalue of > 1.0 were considered as being of interest for interpretation; they were selected, and a Varimax rotation was done to better distinguish which original variables are most correlated with each factor.

Spectral data analysis was done with log (1/reflectance) data. A number of transformations were tested, including standard normal variate, smoothing according to a Savitzky–Golay algorithm, using a first- or second-order derivative, and a first- or second-order polynomial. However, no transformation improved predictions, as raw spectra were characterized by low levels of noise. Partial least-squares (PLS) regressions were computed using the Unscrambler, version 9.2 (Camo Inc., Woodbridge, NJ) to define linear models to predict computed
Correlations among Maturity and Quality Parameters. The various tomato maturity and quality parameters under study are interrelated to a large extent. This reflects the biological evolution of fruit toward maturity and highlights the fact that tomato quality can be described more globally in terms of quality evolution of fruit toward maturity and highlights the fact that are interrelated to a large extent. This reflects the biological factors directly from spectral data. Curve fitting to describe behavior of variables against tomato maturity stage or gustatory index was done using TableCurve 2D (Systat software Inc., Point Richmond, CA).

Equations types were \( Y = (a + bX)^2 \) for Hunter \( L \) and firmness; modified Gaussian for Hunter \( a \) and lycopene; inverted gamma for TCI; \( Y = ax + bx^2 + cx^3 \) for Hunter \( b \); \( Y = a + b \exp(-X/c) \) for SS/TA; and \( Y = a + bx + cx^2 \) for EC and TA.

RESULTS AND DISCUSSION

Correlations among Maturity and Quality Parameters. The various tomato maturity and quality parameters under study are interrelated to a large extent. This reflects the biological evolution of fruit toward maturity and highlights the fact that tomato quality can be described more globally in terms of quality with a multivariate approach.

The surface color of fruit was described using Hunter’s \( L, a, \) and \( b \) scale. Lightness (\( L \)) is inversely correlated with \( a \) (\( r = -0.74 \)) and the \( ab \) ratio (\( r = -0.71 \), Table 1). Hence, as maturation proceeds, \( L \) gradually lowers while \( a \) increases; fruit becomes darker and redder. This is in agreement with a number of previous studies (7, 30, 31). The \( a \) value is of particular interest in tomato because it corresponds to the green—red color axis. The \( b \) value (blue—yellow axis) increases with \( a \) to a certain extent (\( r = 0.51, P < 0.001 \)), but is not related to \( L \), \( r = -0.08 \). The TCI is also inversely related to \( L \), with \( r = -0.86 \). As observed by Gómez et al. (32), a darker tomato has a higher TCI score. On the other hand, TCI and \( a \) are positively correlated (\( r = 0.86 \)). The other color index computed in this study, \( ab \), is highly correlated to the TCI (\( r = 0.95 \)).

Except for Hunter \( b \), color parameters are highly correlated to the other important maturity quality attribute, fruit firmness. Firmness is correlated positively to \( L \) (\( r = 0.78 \)) and negatively to \( a \) (\( r = -0.71 \)), \( ab \) (\( r = -0.67 \)), and TCI (\( r = -0.77 \)).

Regarding the nutritional and gustatory attributes, most color values are correlated to lycopene, pH, and titratable acids, whereas low correlations were observed for soluble solids and EC (Table 1). More specifically, lycopene and pH are positively correlated to \( a \), \( b \), \( ab \) ratio, and TCI and negatively correlated to \( L \). On the other hand, titratable acidity and EC are negatively related to \( a \), \( ab \) ratio, and TCI. In contrast to pH, titratable acids is positively correlated to the \( L \) color value. In our study, neither color values nor fruit firmness is correlated with soluble solids, an important organoleptic attribute of tomato fruit. Soluble solids, however, are positively correlated with titratable acids and EC (Table 1).

Factor Analysis. Fifteen raw variables were used in factor analysis, including color values, firmness, and nutritional and gustatory quality attributes. Four factors were selected, according to the criteria of an eigenvalue of >1.0. These four factors accounted for a large proportion, 81%, of total variance. After computation of a Varimax rotation, it was found that factor 1, with an eigenvalue of 5.42, represented 36.1% of overall variance, followed by factor 2 with an eigenvalue of 2.81 (18.7% of variance). Factors 3 and 4 had eigenvalues of 2.01 and 1.87, respectively, corresponding to 13.4 and 12.5% of total variance.

In our study, factor 1, which we call tomato maturity stage (TMS), is of most interest because it is strongly correlated to Hunter’s \( a \) and \( L \) values, TCI, firmness, lycopene content, and \( ab \) (Figure 1A). These quality attributes have all been related to tomato ripening (10, 33–36). It was expected that maturity would come out as an outstanding factor, because sampling was designed to maximize this specific aspect of tomato quality. Other variables that contribute to TMS are titratable acidity, extract pH, and the SS/TA ratio. On the other hand, variables that do not highly correlate with TMS are EC, Hunter \( b \) color

![Figure 1](http://pubs.acs.org/doi/abs/10.1021/jf072182n)
value, surface pH, fruit weight, and SS (Figure 1A). Whereas SS normally tends to increase with tomato maturity, the increase is not always linear (37). For some cultivars, SS tend to decrease at the deep red stage (38, 39). Hence, SS are a poor indicator of tomato maturity when considering multiple varieties.

TMS being a linear combination of the original parameters included in the model, a maturity score was computed for all fruits in the experiment. It is represented in Figure 1A as plotted against factor 4, called a “variety” factor (VF). To compute a representative TMS, there was a need to cover all possible maturities within our sampling set. Getting fruits exclusively from the market misrepresents very low maturities. The Trust variety, a standard Beef-type tomato, thus formed a basis for model construction, as it is well represented at all maturity levels (“T”, Figure 1B). Fruits collected from the market being more mature, they are positioned at the right of the score plot except for some field-grown fruits (“F”), which were also available at low maturities.

One of the interests of the TMS is that it was obtained from a range of varieties. It is thus possible to use the scale for basically all Beef or Trust tomato varieties on the retail market. The scale, corresponding to the scores obtained from factor analysis, ranges from −2.5 for green fruits to 1.5 for very ripe tomato. The score values can be transformed to a convenient 0−10 scale easily usable by the industry. Using TMS mitigates the problem of current reliance on color to estimate tomato maturity because the lycopene content of fruit, mostly responsible for tomato color, is strongly affected by environmental conditions (12, 40).

Different varieties have a unique physicochemical makeup, which is shown by specific positions on the score plot (Figure 1B). Factor 4 was named ‘variety’ because many of the original variables involved can, to a certain extent, discriminate against varieties. Hunter b, pH, and fresh weight are the three parameters that are most related to VF (Figure 1A). Pink-type tomatoes (“P”) all appear at the lower right end of score plot, as these fruits had a much lower Hunter b color profile as compared to the other fruits (Figure 1B). A large proportion of field-grown tomatoes under study (“F”) have a high VF score; many of them were were higher sized as compared to the greenhouse varieties; they also had a high near-surface pH and Hunter b value. With all scores close to 0 on the VF scale, the Blitz variety (“B”) appears as an average fruit, uniform in terms of fresh weight, Hunter b color, and pH (Figure 1B). VF may not have the same practical interest as TMS, because discrimination of the varieties is only partial, as “Beef” tomato varieties on the market all have similar parents. However, it shows how differences among varieties are handled independently from TMS in factor analysis.

Determination of a TMS from factor analysis allows comparison of the evolution trends of the various raw variables introduced in the model. None of the variables are linearly related to TMS, which suggests that some distortion is expected if any single measurement is used to measure maturity. Hunter a and lycopene are modeled by a Gaussian distribution, whereas TCI increase is best described by an inverse gamma distribution (Figure 2). Both trends are characterized by low increases at the beginning, followed by an exponential increase phase, and finally by a tendency to reach a plateau (Figure 2). Hence, all three variables evolve slowly while tomatoes are still green. Then, probably following the climacteric rise in respiration, the exponential period starts at a TMS of about −2.0 for Hunter a, TCI, and lycopene content. Curve inflection (beginning of the reduced rates of increase) for Hunter a is at a TMS of −0.75; it happens later for TCI (−0.25) and even later for lycopene.

Actually, lycopene increases are almost linear above a TMS score of 0. This outlines the difficulty to predict lycopene content directly from color data. As lycopene content still increases late into the ripening process, Hunter a values are reaching a plateau. Hunter a also cannot discriminate maturity stages of greener tomato (TMS of −2.5 to −2.0; Figure 2). Color scales are meant to mimic human perception and should be used with caution to describe physiological phenomena. Hunter b, measuring the yellow color component, tends to rise, reaches a maximum at a TMS of 0, and then falls. This has also been observed by Arias et al. (41); it is likely due to transient pigment increases or masking of other pigments by lycopene. Hunter L and firmness follow a comparable decrease pattern, with accentuated decrease rates as TMS progresses. With such comparable trends, Hunter L could be used as an estimation of firmness (eq 1), because it shares 63% of firmness variability.

\[
\text{firmness} = 297.4 - 790.4 / \ln (\text{Hunter } L)
\]

\[
r^2 = 0.63 \ (P < 0.01)
\] (1)

Direct assessment of TMS from vis-–NIR spectroscopic data was sought. Results indicate that reliable predictions are possible, because a coefficient of determination \((r^2)\) of 0.93 was obtained (Figure 3A, Table 2). The average prediction error (RMSEP) is 0.26. The ratio of prediction error to standard deviation of data used for calibration (RPD) is 3.86. A ratio above 3.0 is considered to be sufficient for practical applications in spectroscopy (42). Hence, convenient, rapid, and nondestructive measurement of tomato maturity stage, determined on a multivariate basis, is feasible by vis-–NIR spectroscopy.

**Tomato Parameters Related to Taste.** Factors 2 (F2) and 3 (F3) are related to taste. We called F2 the gustatory index (GI) as it is strongly and positively correlated to TA and EC and negatively correlated to pH and SS/TA (Figure 4A). F3 is
strongly correlated to soluble solids, either measured from the homogenate or at the surface, with only limited influences from other variables (Figure 4A). F3 can thus be considered univariate and is simply called soluble solids. Because F2 and F3 are independent, this suggests that no single parameter can account for basic tomato taste. Graphing the GI against SS provides a convenient basis for comparison of fruits and description of taste (Figure 4A). Fruits in quadrant I are most desirable; they have both a high soluble solids content, while being more acid, and a low SS/TA. On the contrary, fruits in quadrant III are less desirable, being less acid, with a low soluble solids content. Because F3 (soluble solids) is univariate and linearly related to Brix readings (eq 2), the limit between low and high ranking can be calculated and corresponds to a value of 4.5.

\[
4.52 + 0.32 \times F3 \text{ score} \quad r^2 = 0.85 \quad (P < 0.001)
\]

All pink-type fruits were located in quadrant II, being high in soluble solids but relatively low in GI. All Blitz fruits (“B”; Figure 4B) were in quadrant III, the less desirable position, with low soluble solids and low GI. Both truss type fruits (“V”) were also in the same quadrant. Although field-grown fruits (“F”) tended to be high in soluble solids, the diversity of varieties and growing conditions probably explains their wide distribution in quadrants I, II, and IV. Trust tomatoes (“T”) were represented in all quadrants, but many fruits ranked high in GI.

The SS/TA ratio decreases with the GI, with steeper decrease rates at the lower end of the GI scale. By contrast, both TA and EC increase with the GI, with a comparable trend (Figure 5). Attempts made to assess taste parameters by means of spectroscopy have not been successful for the GI or for SS (Figure 3B; Table 2). With some sample preparation, SS are conveniently measured by a refractometer. As for the GI, it can be estimated from EC measurement, which is highly correlated both with TA and with GI (Figure 4A). EC is a simple and direct measurement, contrary to TA, which is more tedious to determine. The following equation is proposed to predict the
gustatory index from EC (eq 3). For a GI of 0, EC is 5.4 mS/cm. This is the proposed limit between low and high values for the GI.

\[
GI = 13.55 - 31.31/(EC)^{1/2} \quad r^2 = 0.74 \quad (P < 0.001) \quad (3)
\]

With the factor analysis approach, the population of tomato found on the retail market, as sampled in this study, is divided into four classes more or less equally represented. Whether the limit values of 4.5° Brix and 5.4 mS/cm correlate with organoleptic perception of consumers would have to be tested by sensory analysis. In turn, taste perception will depend on the cultural background of judges and cannot be considered universally objective. Hence, values proposed should be used as a rapid means to compare fruits lots, measure the effect of production practices, or evaluate genetic material.

Our hypothesis was that complex phenomena such as tomato ripening and taste are multidimensional and would be best described by an approach such as factor analysis. We verified robustness of the approach by analysis of nearly 100 fruits representing various Beef and Trust tomato types found on the retail market. This study showed that FI summarizes ripening, and a new variable, called “tomato maturity stage” is proposed. Plotting individual quality parameters against TMS adds to the understanding of the complex relationships among variables. Hunter L and firmness are most linearly related to TMS; Hunter L, being the easiest to measure, may best account for maturity. However, TMS is readily measured directly and nondestructively by means of vis-NIR spectroscopy, with sufficient accuracy for practical use.

These results support more biology-based assessments of tomato maturity and quality, which is largely done by subjective means in inspection systems or by sole use of color, firmness, fresh weight, or size. A better understanding of the underlying variables that describe tomato quality facilitates development of tools that can rapidly measure the impact of various environmental conditions during the growing period and after harvest. The approach can be used for any other fresh produce. The inherent robustness of factor analysis allows input of many variables while handling the problem of multicollinearity. Addition of other physiological measurements, such as respiration rate, would further improve models of TMS.

The proposed two-dimensional taste evaluation scheme could also be used to test the effect of genotype, growing conditions, and postharvest handling. A more global assessment of taste could be obtained by addition of sensory measurement and volatiles/aromas along with the factor analysis approach. Factor analysis also allows consideration of taste independently from maturity.

The spectroscopy results presented in this study were obtained with a laboratory-bench type device, using an integration sphere. Other means to capture the interaction between light and fruits should be explored, such as fiber optic based solid-state spectroscopes with interactance probes. Using such a probe type, Slaughter et al. (43) were actually able to predict tomato soluble solid content with a better accuracy than what was obtained in this study, perhaps because higher incident light intensity better explores internal quality. Possible effects of fruit temperature on calibrations should be investigated.

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