PHYSICOCHEMICAL CHARACTERISTICS AND FINITE ELEMENT SIMULATION OF FIRMNESS IN SOURSOP FRUITS (*Annona muricata* L. cv. Elita) DURING POSTHARVEST

CARACTERÍSTICAS FISICOQUÍMICAS Y SIMULACIÓN DE LA FIRMEZA POR ELEMENTOS FINITOS DE FRUTOS DE GUANÁBANA (*Annona Muricata L. cv. Elita*) EN POSCOSECHA

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ABSTRACT: Soursop fruits (*Annona muricata* L. cv. Elita) at different ripening stages were evaluated for their physicochemical characteristics: total soluble solids (TSSs), acidity, and pH. Firmness was determined through the application of puncture textural tests. The modeling and simulation of this parameter was carried out on Autodesk Inventor Professional 11.0 (ANSYS® Technology). The fruits showed an upward trend regarding TSS and acidity, reaching maximum values of 12.8 °Brix, 0.74% acidity, and a pH below 3.43; all of which coincide with consumption maturity as observed on day 6. Firmness showed a decreasing trend throughout the entire postharvest period, with values of 79.43 N for day 0, and 3.62 N for day 9. Finite element modeling, the simulation of firmness, and its correlation with experimental data allowed for us to calculate the fracture force of the fruits with an exactness of more than 90%. Since it prevents the physical alteration of the product, this application becomes a nondestructive alternative for firmness assessment, useful in storage, transport, fresh consumption, packaging, and processing.

KEYWORDS: Tropical fruits, texture, ripening, rheology

RESUMEN: Frutos de guanábana (*Annona muricata* L. cv Elita) en diferentes etapas de maduración fueron evaluados, determinando sus características físico-químicas: sólidos solubles totales (SST), acidez y pH. La firmeza se encontró mediante la aplicación de pruebas de penetración uniaxial. El modelado y la simulación de la firmeza se llevó a cabo por el software Autodesk Inventor Professional 11.0 (ANSYS® Technology). Los frutos mostraron una tendencia creciente con respecto a los SST y la acidez, alcanzando valores máximos de 12,8°Brix y acidez de 0,74%, y un pH inferior a 3,43, valores que coinciden con la madurez de consumo, tal como se observa para el día 6. La Firmeza mostró una tendencia decreciente durante todo el período de poscosecha, con valores de 79,43 N para el día 0 y 3,62 N para el día 9. La simulación por elementos finitos de la fuerza de firmeza presentó alta correlación (>90 %) con respecto a los datos experimentales. La simulación por elementos finitos se convierte en una alternativa no destructiva para la evaluación de la firmeza, útil para el almacenamiento, transporte, consumo en fresco, envasado y procesamiento de éstas frutas.

PALABRAS CLAVE: Frutas tropicales, textura, maduración, reología

1. INTRODUCTION

Soursop fruit can be considered to be promising for the international market due to its excellent nutritional and organoleptic characteristics. However, because of its structure, it can easily get damaged, inducing changes in texture and physicochemical conditions that, in turn, limit its shelf life and reduce its quality when stored inappropriately [1]. The textural and rheological properties of fruits are important attributes that influence their overall quality, storage and processing conditions, acceptability on the part of consumers, transportation, design, optimization, and selection of equipment [2–5]. One of the major characteristics that define the internal and external quality of a fruit is firmness [6]. The evolution of this feature accompanies the different ripening stages in conjunction with a series of physicochemical characteristics such as color, flavor, and aroma, among others [7–8].

The finite element method (FEM) is a numerical procedure currently applied to many engineering problems whose complex formulation does not allow exact solutions. This technique combines a series of mathematical concepts to produce systems of linear and nonlinear equations, whose solution is based on computational techniques [9]. It has been used in the analysis of mechanical stress in various agricultural products, thus allowing for the modeling of irregular geometry objects [10–13].

In this context, the aim of the present study was to relate the finite element simulation of postharvest fruit firmness evolution to a series of physicochemical characteristics such as total soluble solids (TSSs), acidity, and pH.

2. MATERIALS AND METHODS

Plant material. The present research was carried out on soursop fruits obtained from local commercial farm. All the fruits were harvested at the same ripening point, and on the same day, transported in styrofoam boxes to the facilities of the National University of Colombia, Medellin campus, for their corresponding analysis. The experiments of mechanical characterization were conducted under laboratory conditions. The equipment used to measure fruit firmness was a TA-XT2i® texture analyzer equipped with Texture Expert Exceed 2.64 software (Stable Micro Systems Ltd., Godalming, UK).

2.1. Physicochemical characterization

Total soluble solids (TSS, expressed in °Brix) was measured by refractometry [14] at a temperature of 23 °C, on Leica Auto Abbe equipment with a 0–32% measuring range. *Acidity* was obtained by potentiometric titration acid-base reaction, and expressed as percentage of malic acid). The *pH* was determined with a CG-840B Schott potentiometer [15].

2.2. Mechanical characterization

The experimental firmness force was determined graphically from the maximum strength needed to penetrate the fruit, as applied immediately before a sudden force decrease resulting from deformation [16]. This parameter was measured with a 5 mm diameter, flat ended, stainless steel probe, at a loading rate of 2 mm•s^{-1} attached to a TA-XT2 Texture Analyzer.

Firmness simulation. Finite element simulation and modeling was carried out on Autodesk Inventor Professional 11.0 (ANSYS® Technology). In order to use this software tool, it was necessary to determine the physical properties of the material studied: the density, Poisson's ratio, Young's modulus, and the elastic limit.

Density. This variable was assessed on 6 experimental units every day during the postharvest period. Each fruit was weighed to obtain its mass. The volume was determined by applying Archimedes' principle, using water at 25 ^{o}C as the reference liquid. The following relation was used to calculate the density of the fresh plant material:

$$\rho = \frac{M}{V}$$

Where: ρ = density (kg/m^3); M = mass (kg); V = volume (m^3).

Poisson's ratio (μ). This feature was determined for 6 experimental units every day during the postharvest period. The fruits were subjected to unidirectional compression using a TA-XT2 texture analyzer equipped with a 50 kgf load cell (loading rate of 2 mm•s^{-1}) and a 150 mm diameter platen. Resting on their peduncle, the fruits received uniaxial compression force applied on the apical end, and thus exerted along their longitudinal axis. Lateral and longitudinal deformation undergone by the fruits was measured with a 0.001 mm resolution. Poisson's ratio was calculated from the following relation [17]:

$$\mu = -\frac{\frac{\Delta D}{D}}{\frac{\Delta L}{L}}$$

Where: μ = Poisson's ratio (dimensionless); ΔD = lateral deformation (m); D = initial width (m); ΔL = longitudinal deformation (m); L = initial length (m)

Young´s modulus (E). This was obtained assuming that the viscoelastic nature of the fruit does not become manifest for small load times. According to reference [18] the impossibility of expressing the results of compressive load tests applied on highly heterogeneously shaped objects (such as convex soursop fruits) leads to report deformation curves in terms of force versus deformation, instead of stress versus deformation. Applying the theory of contact stress, the following relation was used to evaluate the elasticity modulus of the fruits, provided that the loading probe is a cylindrical rod with rounded ends of curvature diameter “d” [19].

$$E = \frac{0.531F(1-\mu^2)}{D^{\frac{3}{2}}}\left[\frac{4}{d}\right]^{\frac{1}{2}}$$

Where: E = modulus of elasticity (N/m^2); F = force (N); μ = Poisson’s ratio (dimensionless); D = the deformation of the material’s elastic zone (m); d = average curvature diameter of the cylindrical load probe (m).

The force and deformation values used to calculate the modulus of elasticity (E) were defined only up to the point of inflection of the resulting curve. This inflection point was found by changing the sign of the second derivative of the function [20]. In this way, the shape changes undergone by the fruit are not modeled as total deformation, thus allowing for a valid and successful application of the theory of solid mechanics [18].

3. RESULTS AND DISCUSION

3.1. Physicochemical characterization

Figure 1A shows TSS least significant differences (LSDs) as a function of postharvest time. The analysis of variance (ANOVA) shows that there is a significant effect of postharvest time ($P < 0.05$). A rapid TSS increase can be observed from day 1, reaching a peak (12.8 °Brix) on day 6, which corresponds to the CO2 production peak of a typical climacteric fruit. This demonstrates the high α and β amylase metabolic activity that, during maturation, hydrolyzes starch to simple carbohydrates such as disaccharides and monosaccharides (mainly sucrose, glucose, and fructose [21]. The TSS levels found in the present work are consistent with the results of [22] who found ripe soursop fruit concentrations of 13 °Brix. In this regard, the Colombian Technical Standard (NTC) 5208 establishes minimum TSS values of 13.5 °Brix for soursop at consumption maturity; which is slightly higher than the 12.8 °Brix value found in this work, that is, in turn greater than the one found by [23] for other soursop cultivars.

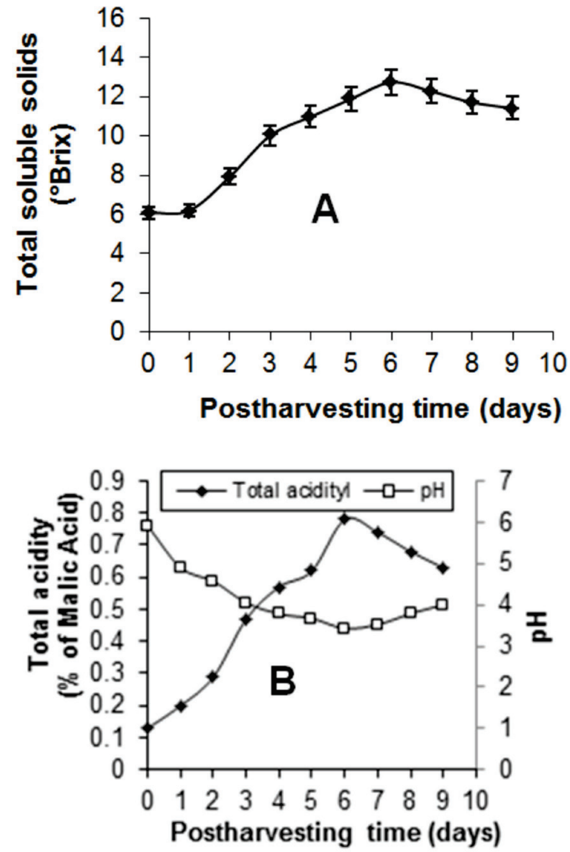

Figure 1.A. TSS behavior in soursop fruits (*Annona muricata* L. cv. Elita) stored at 23 °C and 65% RH; **B:** Changes in total acidity and pH of soursop fruits (*Annona muricata* L. cv. Elita) stored at 23 °C and 65% RH during postharvest

Both total acidity expressed as malic acid concentration (%) and pH are shown in Fig. 1B, which presents their LSDs. According to ANOVA, postharvest time has a significant effect on both factors ($P < 0.05$). Figure 1B shows an increase in total acidity throughout the climacteric stage, reaching a maximum of 0.74% on day 6 of postharvest, and a consequent decrease in pH coinciding with consumption ripeness. According to the values found, soursop could be classified as an intermediate acidity fruit [24]. In the postclimacteric stage, which begins on day 6, the decrease in acidity may be due to the consumption of these organic molecules in various metabolic cycles, in order to provide the energy required by the fruit. In addition, many organic acids are involved as precursors of volatile substances, which enhance their presence during this period [25]. The values for total acidity are slightly lower than those reported by [26]. The acidity values found here meets NTC 5208.

3.2. Mechanical characterization of firmness force

The assessment of firmness, expressed as maximum penetration force (N) is shown in Fig. 2. The ANOVA reveals postharvest time has a significant effect ($P < 0.05$) on this factor.

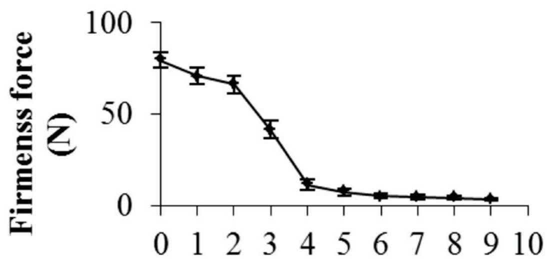

Figure 2. Effect of postharvest time on firmness of soursop fruits (*Annona muricata* L. cv. Elita) stored at 23 °C and 65% RH

Figure 2 shows how fruit firmness is largely variable in this case. With an average of 80 N, unripe fruits (day 0) are very resistant to penetration, even until day 2 after harvest. Between days 2 and 4, we could observe the fastest firmness decrease, which slowed down since day 4, showing a gentle slope that yielded ripe fruit values of 7.48 N and 4.72 N on days 5 and 7, respectively. Overripe fruits (day 9) show an average of 3.62 N, which indicates an extremely soft tissue. In general, the behavior observed in this parameter coincides with the one reported by [16] Firmness records of 60 N at harvest have been observed for other soursop cultivars, followed by a similar behavior to the one observed in the present work during the remaining period [26]. Cell wall changes are the result of the hydrolysis of pectic compounds by the action of pectin methylesterases, polygalacturonases, and cellulases acting on high molecular weight polymers such as cellulose and hemicellulose. It is worth mentioning that the reduction in cell turgor due to transpiration can ultimately reduce firmness [27].

Multiple regression was applied to establish the relationship between fruit physicochemical features and flesh firmness. At a confidence level of 95%, the ANOVA showed that there was a significant effect of TSS, acidity, and postharvest time on flesh firmness. The following fitted model was obtained with a 95% adjustment regression coefficient**.** According to the model, fruit firmness has a negative correlation with postharvest time, indicating that this parameter decreases during ripening; a situation already evidenced by [8].

$$F = B1 - B2 * A - B3 * TSS - B4 * T$$

Where B1 = 116.77, B2 = 32.944, B3 = 5.19, and B4 = 3.54. A is the acitity in %, TSS is total soluble solids in °Brix, T is the time in days, and F the firmness force in Newtons.

3.3. Modeling and simulation of fruit firmness

Table 1 shows the average results obtained for the studied mechanical properties: density, Poisson's ratio, Young's modulus, and the elastic limit as recorded daily during the studied postharvest period. These measurements were used both to characterize the studied material and as the input of the Autodesk Inventor Professional 11.0 software, so as to model and simulate postharvest fruit firmness.

Table 1. Mechanical properties of soursop fruits (*Annona muricata* L. cv. Elita) stored at 23 °C and 65% RH

Day	Density ($g \cdot cm^{-3}$)	Poisson's ratio (Dimensionless)	Young's module (GPa)	Elastic limit (MPa)
0	0.982±0.016	0.4±0.038	$1.16 \cdot 10^{-3}$	$1.86 \cdot 10^{-2}$
1	0.986±0.023	0.4±0.045	$1.03 \cdot 10^{-3}$	$1.65 \cdot 10^{-2}$
2	0.989±0.022	0.41±0.041	$9.62 \cdot 10^{-4}$	$1.54 \cdot 10^{-2}$
3	0.991±0.032	0.42±0.039	$6.03 \cdot 10^{-4}$	$9.6 \cdot 10^{-3}$
4	0.996±0.014	0.43±0.043	$2.29 \cdot 10^{-4}$	$3.7 \cdot 10^{-3}$
5	0.997±0.042	0.43±0.031	$1.04 \cdot 10^{-4}$	$1.3 \cdot 10^{-3}$
6	0.998±0.052	0.43±0.033	$8.12 \cdot 10^{-5}$	$1.3 \cdot 10^{-3}$
7	1.007±0.029	0.45±0.054	$8.12 \cdot 10^{-5}$	$1.3 \cdot 10^{-3}$
8	1.013±0.041	0.47±0.040	$8.10 \cdot 10^{-5}$	$1.21 \cdot 0^{-3}$

Table 1 shows how the density of the studied soursop fruits underwent a slight increase with ripening, accentuated during over-ripening. This may be due to the flow of the gaseous fraction from the inner spaces of the material to the outside, which causes it to become more compact, and slightly increases its density

[28]. Evaluated daily during storage, Poisson's ratio increased with ripening, as it can be seen through the greater lateral (ΔD) to longitudinal (ΔL) deformation of the fruit. Since firmness decreases with ripening, Young's modulus decreased along postharvest. Similar results were found in Fuyu persimmon and Golden Delicious apple fruits [19,29]

According to reference [18] the elastic limit is a theoretical value that, in the present case, followed the behavior of Young's modulus during the entire period studied. Figure 3 shows the obtained finite element tetrahedral solid meshing and the results of failure analysis under penetration loading as simulated with the Autodesk Inventor Professional 11.0 software, based on the mechanical property data recorded.

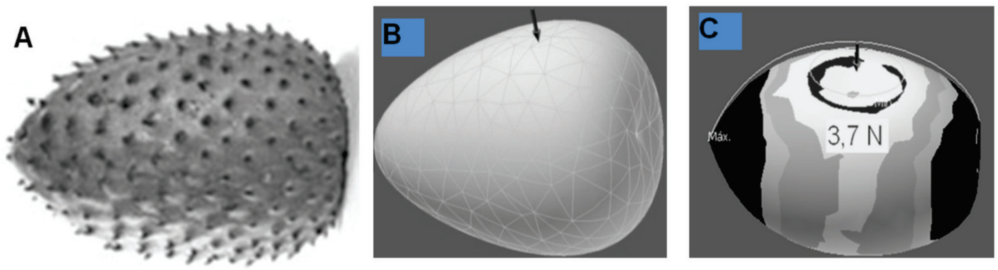

Figure 3. Soursop fruit (*Annona muricata* L. cv. Elita): A. original product; B. geometric volume generated by the creation of a surface of revolution and meshed with tetrahedral finite elements; the arrow indicates the load application point; C. modeling and simulation of the penetration force applied on soursop fruit

According to the safety factor criterion (Fig. 3C), the highest probability of failure occurs in areas in which, under the influence of the penetration load, stress is more widely distributed. It can also be observed that failure stress tends to decrease along the ripening process, a situation that is related to cell wall degradation resulting in turn from the hydrolysis of pectic compounds and high molecular weight carbohydrates [30].

Table 2 presents the experimental and simulated rupture maximum force average values obtained for soursop fruits in the present work together with the corresponding safety factor, all assessed on a daily basis during the postharvest period studied.

Table 2 reveals an excellent fitness between experimental and simulated data, thus indicating that the assessed mechanical properties, as well as the selected mesh and elasticity criteria, were optimal for defining the mechanical response of the material studied. The greater discordance between modeled and experimental values could be observed in unripe and half-ripe fruits, probably due to the necessary assumptions made on the initial conditions of the material studied, especially those regarding it as an isotropic solid throughout which stresses are uniformly distributed. Finite element simulation of compression stresses in other fruits has rendered similar effort distribution results [31]. The safety factor results were consistent with the provisions of the theory of failure (also known as the Von Mises-Hencky theory), which states that the safety factor must be less than one. This concept is applied as a failure criterion for materials [32].

Table 2. Experimental and (finite element) simulated rupture maximum force values and corresponding firmness safety factor for soursop fruits (*Annona muricata* L. cv. Elita) stored at 23 °C and 65% RH

Day	Experimental force (N)	Simulated force (N)	Safety factor
1	79.43	75	0.862
2	70.74	65	0.884
3	66.13	60	0.884
4	41.56	40	0.844
5	11.46	14	0.856
6	7.48	7	0.835
7	5.27	5	0.916
8	4.72	5	0.918
9	4.42	4.5	0.920

4. CONCLUSIONS

The soursop fruit (cv. Elita) physicochemical quality values found in the present study regarding TSS, total acidity (expressed as malic acid), and pH were observed to be within the limits recommended by the NTC for this crop (NTC 5208). However, the TSS record was found to increase during ripening and until over-ripening, when there was a slight decrease, probably due to the onset of fermentation processes.

Fruit firmness registered a minimum and a maximum on days 0 and 9 of postharvest, respectively, showing a steady decrease trend that reached its maximum slope between days 2 and 4. Within the mechanical properties evaluated, it is important to highlight the decrease in Young's modulus, the increase in density, and Poisson's ratio along ripening. These mechanical properties are necessary for finite element modeling and the simulation of firmness. This is a non-destructive technique that allows us to estimate this important parameter during postharvest without physically altering the product.

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