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Determination of geometric properties of cocoa beans (*Theobroma cacao* L.)

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ABSTRACT
Objective: To determine the linear physical dimensions of dried Mexican cocoa beans to estimate their geometric properties and differentiate them through a principal component analysis.
Design/Methodology/Approach: For the research, 51 dry samples of cocoa beans (*Theobroma cacao* L.) were collected from three producer states in Mexico. The physical properties of cocoa beans were determined based on their linear dimensions: length, width, thickness, geometric diameter, sphericity, volume, and shape factor. Moisture, average weight, and ether extract were also determined.
Results: The results revealed the relation between linear and geometric properties, particularly the fact that bean weight is significant ($p<0.001$) regarding all the properties evaluated, except moisture. Said relation explained 98.8% of the total variation in the first two components observed in the cocoa samples from the three states (Tabasco, Chiapas, and Oaxaca). Average bean weight, sphericity, and volume contributed the most to the total variation.
Findings/Conclusions: The only quantitative variable that showed significance was bean weight. The other measurements —length, width, and thickness— did not. However, there was significance when coupling the measurements in the expressions of surface area and volume.

Keywords: Geometric properties, Cocoa beans, Main components.

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INTRODUCTION

Cocoa beans are the prime raw material in the chocolate and confectionery industry. The preparation of cocoa beans depends on local customs and industrial processing. Based on the postharvest treatment, beans harvested in Mexico can be classified as washed-dried or fermented-dried (NMX-FF-118-SCFI-2014). Fermentation is the essential process to produce the particular sensory characteristics of cocoa. However, even today, the many factors involved in said process rely on traditional practices lacking controlled procedures (Saltini *et al.*, 2013; Alvarez-Villagomez *et al.*, 2022). Drying is the final stage of preparation,

its main objective being to reduce moisture to a microbiological and physicochemical safety value and to cut down the acidity generated during fermentation (Afoakwa, 2014; Saltini *et al*., 2013; Arana-Sánchez *et al*., 2015). Both fermentation and drying influence the original chemical composition through microbial, enzymatic, and chemical activity, also reflected in structural and physical changes in cocoa beans. According to García-Alamilla *et al*. (2012), in the case of cocoa, physical properties have great relevance, with the main characteristics that reflect postharvest phenomena being the length, width, thickness, and average weight of beans. In addition, these features are also indices of commercial importance and industrial processing.

Various studies have evaluated the size and shape of cocoa beans based on basic measurements (Bart-Plange and Baryeh, 2003; Aosiro *et al*., 2020). Such data contribute to selecting and improving cultivars, managing the supply chain, and designing equipment. It also assists in the electrostatic separation of contaminants (Manfreda and Acosta, 2014; Aosiro *et al*., 2020) and provides relevant variables for the bean drying unit operation. Although bean size has been a meaningful indicator for other crops, in the case of cocoa beans there is no adequate study defining the role of size. We therefore need more studies to evaluate the size-embryo ratio, just as Manfreda and Acosta (2014) reported for cereals. Bean size and its relation to surface area have an impact on fermentation due to the diffusion and hydrolysis processes that occur between the mucilage and the cotyledon. Moreover, roasting is the first step of industrial transformation after the postharvest stages, so that if bean size presents high variability and there is no adequate classification, there may be cocoa batches with under-roasted or over-roasted beans. Therefore, the objective was to determine the linear physical characteristics of dried Mexican cocoa beans to estimate their geometric properties and differentiate them through a principal component analysis.

MATERIALS AND METHODS

Study site selection and sampling

The study sites selected were representative of the states of Tabasco and Chiapas as the main cocoa producers in Mexico (SIAP, 2022). The state of Oaxaca was also included. The samples were collected from December 2021 to March 2022. Cocoa producers contributed samples of both washed-dried and fermented-dried beans. A total of 51 samples were collected: 36 from Tabasco (16 from Comalcalco, six from Paraíso, six from Huimanguillo, four from Cunduacán, two from Cárdenas, one from Jalapa, and one from Teapa); 12 from Chiapas (five from Pichucalco, two from Ostuacán, two from Tecpatán, one from Salto de Agua, one from Huixtla, and one from Ignacio Allende); and three from Oaxaca (two from Toltepec and one from Puerto Escondido). Each sample weighed approximately one kilogram.

Assessed variables

Moisture

An average of 10 cocoa beans were taken and placed in the Aqua Boy KPM202 moisture content meter (Germany) with direct reading.

Ether (fatty) extract

The ether extract was determined using the methodology according to the NMX-F-615-NORMEX-2018 Food –determination of ether extract (soxhlet method) standard.

Average bean weight

The average bean weight was determined based on the random quantification of 100 beans' weight, using a semi-analytical balance (Ohaus, Scout Pro SP202, China) with an accuracy of 0.01 g. To obtain the average weight, the recorded weight was divided by 100 (Afoakwa *et al.*, 2014).

Linear and geometric bean dimensions

The sample (60 grains) was taken at random to determine the length (L), width (W), and thickness (T) of each bean. The length was measured in millimeters using a digital vernier caliper (KNOVA, China) as per the description provided by Kaushik *et al.* (2007). Width and thickness were measured perpendicularly to the long axis (Bart-Plange *et al.*, 2003; Oyedokun *et al.*, 2011; García-Alamilla *et al.*, 2012; Jaiyeoba *et al.*, 2016; Sandoval *et al.*, 2019). The sphericity degree was calculated using equations (2) and (3) as described by Bart-Plange *et al.* (2003), Jaiyeoba *et al.* (2016), Kwino *et al.* (2017), and Sandoval *et al.* (2019).

$$\Phi = \left(\frac{WTL}{L}\right)^{1/3} \quad (1)$$

$$\Phi = \left[\frac{B(2L-B)}{L}\right]^{1/3} \qquad B = (WT)^{0.5} \quad (2)$$

Geometric diameter

The geometric mean diameter was calculated using the expression cited by Bart-Plange *et al.* (2003), García-Alamilla *et al.* (2012), Jaiyeoba *et al.* (2016), and Sandoval *et al.* (2019).

$$D_g = (WLT)^{1/3} \quad (3)$$

Where: D_g is the geometric mean diameter (mm).

It becomes evident that the sphericity from equation (1) is a function of D_g and therefore:

$$\Phi = \frac{D_g}{L} \quad (4)$$

Surface area

The surface area was calculated using the mathematical expression given by Bart-Plange *et al.* (2003), García-Alamilla *et al.* (2012), Jaiyeoba *et al.* (2016), and Sandoval *et al.* (2019).

$$S=\frac{\pi BL^2}{2L-B} \quad (5)$$

Where: S is the surface area.

The surface area was estimated based on the D_g and using the expression posited by McCabe, Smith, and Harriott (Bart-Plange *et al.*, 2003):

$$S=\left(\pi D_g\right)^2 \quad (6)$$

Volume

The volume was calculated using the mathematical expression given by García-Alamilla *et al.* (2012):

$$V=\frac{\pi B^2 L^2}{6\left(2L-B\right)} \quad (7)$$

Shape factor

Cocoa bean is considered an ellipsoid of revolution, and its shape factor is estimated as follows:

$$Fm=\frac{1}{2}\left(\frac{L}{D_g}\right)^{1/3}\left(\frac{D_g}{L}+\frac{L}{e}Arcsen\left(e\right)\right) \quad (8)$$

Considering the shape factor, the surface area is estimated as follows:

$$S=\frac{3\left(1-\varepsilon\right)}{D_g}\left(\frac{D_g}{L}+\frac{1}{e}Arcsen\left(e\right)\right) \quad (9)$$

$$e=\sqrt{\frac{L^2-D_g^2}{L^2}} \quad (10)$$

And the estimated volume as follows:

$$V=\frac{\pi D_g^2 L}{6} \quad (11)$$

Data processing and statistical analysis

Descriptive statistics were conducted for all evaluated variables and a principal component analysis (PCA) was implemented. The PCA was performed using standard deviations, the Pareto scaling method, and a Pearson correlation analysis with MetaboAnalyst 5.0.

RESULTS AND DISCUSSION

The size and the number of beans per 100 g are two relevant indices for measuring the physical quality of cocoa beans (Kongor *et al.*, 2016). Another significant factor is bean moisture, which should be 7%, since a higher percentage leads to deterioration due to the presence of microorganisms (fungi), and less than 6% turns the beans brittle (Andrade-Almeida *et al.*, 2019). Table 1 shows the average values of all samples, of both washed-dried and fermented-dried cocoa beans. The general evaluation of physical measurements in all samples shows the variability between commercialized beans. These variations are associated with different factors, such as genetics, edaphoclimatic conditions, and postharvest treatment. As we already mentioned, the moisture variable is critical. Regarding the samples in this study, moisture reached 5.24% (Table 1) with a deviation slightly higher than 24%, which is above the permissible limits, making the beans susceptible to microbial contamination.

The visual appearance of cocoa beans is meaningful because it determines handling in the postharvest treatment (fermentation and drying), which will ultimately impact flavor, an essential quality in cocoa beans (Sánchez *et al.*, 2017). For example, authors such as Álvarez *et al.* (2007) argue that the average weight of fermented and dried cocoa beans is linked to their shell content (*testa*). Moreover, weight affects the fat yield. The results showed a variability of approximately 20% (Table 1) in the average weight, which has different causes. Among these are moisture (which is not homogeneous between the samples), genetics, and postharvest handling. Some samples were washed-dried, and others fermented-dried. When the fermentation process does not adequately degrade the mucilage, the weight of the beans is greater than that of a washed sample, which is reflected in the percentage of shell content (*testa*). We must consider that cell walls in fermented beans are destroyed, which exposes beans to chemical factors that affect their properties, including organoleptic ones (Vera *et al.*, 2014). The fat content was 49% on average, with moderate variation.

Various authors have evaluated the linear dimensions of cocoa beans (Bart-Plange and Baryeh, 2003; Álvarez *et al.*, 2007; Oyedokun *et al.*, 2011; García-Alamilla *et al.*, 2012; Andrade-Almeida *et al.*, 2019) using native or improved commercial varieties and different approaches in their research. Bart-Plange and Baryeh (2003) and Andrade-Almeida (2019)

Table 1. Physical properties of Mexican cocoa beans.

Physical characteristics of the grain	Means	Max	Min	±SD	CV (%)
Moisture (%)	5.24	9.1	2.4	1.30	24.93
Average weight 100 beans (g)	112.96	202.3	71.3	22.30	19.74
Butter (%)	49.66	75.13	27.34	6.70	13.48
Length (mm)	21.54	25.56	17.19	101.66	8.72
Width (mm)	12.65	21.27	8.72	1.22	9.64
Thickness (mm)	7.34	9.46	5.99	0.73	9.93
LB/TB	2.94	3.69	2.17	0.27	9.44

Source: compiled by authors.

worked with African and South American cocoa beans (ICS, CCN51) and obtained an average weight higher than the one registered in the present research. This research has no specific genetic variety, but rather commercial beans presenting native materials and unidentified crossbreeds. However, the evaluated samples included washed and dried cocoa beans, unlike those reported by the abovementioned authors, who used only fermented beans. As stated above, moisture is a critical value for the linear dimensions and the average weight. Vera *et al.* (2014) studied fermented samples from 15 clones in Ecuador and reported an average weight of 136 g for 100 beans, with a moisture of 6.49%. In the present study, the average moisture was 5.1%. Likewise, Álvarez *et al.* (2007) reported a moisture between 4.26% and 6.37% for the genotypes they evaluated and 5.17% for a commercial sample. Additionally, these same authors reported a fat content between 54.61% and 56.07% for the different genotypes and 56.01% for the commercial sample, higher values than those reported in the present study.

Running the linear dimensions of the cocoa beans through equations 1 to 11 allowed us to estimate the geometric diameter, sphericity, surface area, volume, and shape factor (ellipsoid of revolution). The results are presented in Table 2. The work conducted by Oyedokun *et al.* (2011) maintains that linear dimensions are linked to the cocoa variety and that morphology indicates quality, yield, and pest resistance or susceptibility while in storage. The shape, surface area, volume, and size of cocoa beans depend specifically on the amount of stored water —the more water contained, the greater the dimensions (García-Alamilla *et al.*, 2012). To determine sphericity, one must assess to what extent the object under observation resembles a sphere, which impacts its tendency to roll —something particularly relevant in agricultural products. This property is helpful in the design of hoppers and husking equipment (García-Alamilla *et al.*, 2012; Jaiyeoba *et al.*, 2016). To estimate sphericity and surface area, two sets of equations were used (equations 1 and 2; and equations 5 and 6, respectively). The results show that cocoa beans do not resemble a sphere. Still, regarding the shape factor (using equation 8), the cocoa beans coincided with an ellipsoid of revolution, as shown in Table 2. The geometric dimensions obtained from the linear dimensions were greater than those reported by Bart-Plange and Baryeh (2003). When compared to the results of García-Alamilla *et al.* (2012), the averages were lower for surface area (1006.99-890.48 mm^3) and volume (1280.17-873.76 mm^3). In the case of Sandoval *et al.* (2019), the geometric dimensions of fermented Trinitario beans are above those recorded in the present study, with a geometric diameter of 15.9 mm, a surface area of 742.4 mm^2, and a sphericity of 0.61. The results for each variable, one may infer, are related to very particular characteristics: edaphoclimatic conditions, plantation age, plantation management, distribution, and biodiversity. Concerning said characteristics, through an (unreported) questionnaire, for the most part, a density of 614.09 trees/ha, a productivity of 649-695 kg/ha, an average age of 31 years with a majority of young replantings, and biodiverse plantations were observed. The producers implement good practices, and few of them use agrochemicals. As reported by the producers, the genetic origin of the samples in ascending order was Trinidadian, foreigner, Creole, and clones.

Table 2. Average geometric properties.

Properties	Means	Max	Min	±SD	CV (%)
Sphericity (equation 1)	0.58	0.65	0.50	0.03	4.44
Sphericity (equation 2)	2.46	2.66	2.31	0.06	2.46
Dg (mm) (equation 3)	12.55	15.17	10.66	0.91	7.22
Surface area (mm^2) (equation 5)	420.23	609.51	306.99	59.70	14.21
Surface area (mm^2) (equation 6)	498.30	724.04	365.37	71.03	14.25
Volume (mm^3) (equation 7)	681.39	1195.50	436.77	146.20	21.46
Shape factor (equation 8)	1.04	1.089	1.022	0.008	0.83
Surface area (equation 9)	0.22	0.27	0.18	0.01	7.45
Volume (equation 11)	1816.35	3372.62	959.25	405.78	22.34

Source: Compiled by authors.

Table 3 shows the correlation between the physical variables of the commercial samples from the three states (Tabasco, Chiapas, and Oaxaca). The correlation analysis showed that the length of the dried beans was significant ($p \leq 0.0001$) regarding all the physical variables and the equations where it partakes, except moisture. The sphericity resulting from equations 1 and 2 indicates the extent to which the bean shape resembles a sphere —which was not the case for cocoa beans. Meanwhile, the shape factor obtained with equation 8 better represents the morphology of the bean as an ellipsoid, which was positively correlated ($p \leq 0.0001$) to bean length and negatively to bean thickness and width, which are part of the geometric diameter estimation. Bean weight was not dependent on moisture, shape factor, or sphericity (equation 1), but it was highly significant ($p \leq 0.001$), whether positively or negatively, for all other variables. The volume estimated through equation 9 was the variable most correlated to the rest, except for the bean's L/E ratio and the shape factor (equation 8). In all cases, moisture —already cited as a critical variable— did not show a correlation either with the linear measurements or with the results derived from the equations.

The PCA explained 98.8% of the total variation observed for the first two components in the samples from the three states (Tabasco, Chiapas, and Oaxaca). No outliers were observed.

The first principal component (PC1) explained 96.8% of the total variation, with bean weight, surface area (equations 5 and 6), and volume (equation 7) being the major contributors (Table 4). For this component, all significant variables presented a negative correlation. The second principal component (PC2) explained 2% of the total variation, with bean weight, bean length, surface area (by equations 5 and 6), volume (equation 7), and shape factor being the variables that described this variation. The positive contribution came from the area and volume equations.

Figures 1 and 2 contain the graphs from the PCA (scores and loadings), showing the weight of the two main components obtained with the standard deviations. The score graph shows the discrimination and classification of the assessed physical properties according to the data matrix of 51 samples. It also shows similarities between the groups. The pattern of

Table 3. Correlation of physical variables of cocoa beans from three Mexican states (Tabasco, Chiapas, and Oaxaca).

	LB	Eq. 7	Eq. 2	Eq. 6	Eq. 3	Eq. 5	ABW	Eq. 11	WB	TB	LB/TB	Eq. 8	Eq. 9	Eq. 1	Moisture
LB	1														
Eq. 7	0.7156*	1													
Eq. 2	0.7873*	0.9812*	1												
Eq. 6	0.7949*	0.9910*	0.995*	1											
Eq. 3	0.8075*	0.9839*	0.9982*	0.9983*	1										
Eq. 5	0.8075*	0.9887*	0.9938*	0.9996*	0.9982*	1									
ABW	0.7431*	0.7971*	0.8081*	0.8200*	0.8184*	0.8231*	1								
Eq. 11	0.8998*	0.9456*	0.9643*	0.9761*	0.9858*	0.9803*	0.8375*	1							
WB	0.4569*	0.8080*	0.7601*	0.7731*	0.7612*	0.7692*	0.5461*	0.7003*	1						
TB	0.4870*	0.8110*	0.8161*	0.8017*	0.8040*	0.7950*	0.6490*	0.7252*	0.03796*	1					
LB/TB	0.4322*	-0.1607**	-0.1062	-0.0844	-0.0747	-0.0657	0.0300	0.0910	0.0329	-0.5732*	1				
Eq. 8	0.5612*	-0.1601**	-0.0657	-0.0499	-0.0318	-0.0279	0.1120	0.1562	-0.2737*	-0.3085*	0.8464	1			
Eq. 9	-0.8864*	-0.9330**	-0.9792*	-0.9713*	-0.9815*	-0.9742*	-0.8137*	-0.9769*	-0.6931*	-07536*	-0.0524	-0.1264	1		
Eq. 1	-0.5691*	0.1545	0.0495	0.0400	0.0205	0.0198	-0.1146	-0.1654*	0.2745*	0.3007*	-0.8442*	-0.9953*	0.1418	1	
Moisture	-0.0433	0.0460	0.0192	0.0290	0.0202	0.0268	-0.0261	0.0149	0.0644	0.0221	-0.0647	-0.1051	0.0110	0.1009	1

ABW: Average Bean Weight; length (L), WB: Width Bean; TB: Thickness Bean; ratio LB/TB

Table 4. Principal component analysis of cocoa beans physical properties.

Variable	CP1	CP2	CP3
ABW (g)	-0.1494*	-0.1686*	0.9722*
LB (mm)	-0.0437	-0.1792*	-0.0426
WB (mm)	-0.0308	0.1062	-0.0277
TB (mm)	-0.0246	0.0671	0.0327
Ratio LB/TB	-0.00003	-0.1068	-0.0336
(eq 3)	-0.0359	0.0211	-0.0031
(eq 1)	0.0003	0.0434	0.0089
(eq 2)	-0.0091	0.0072	-0.0006
(eq 5)	-0.2967*	0.1699*	-0.0207
(eq 6)	-0.3230*	0.2299*	-0.0137
(eq 7)	-0.4629*	0.7107*	0.0574
(eq 8)	-0.0001	-0.0231	-0.0044
(eq 9)	0.0047	0.0023	0.0016
(eq 11)	-0.7523*	-0.5668*	-0.2116*
Moisture (%)	-0.0010	0.0319	-0.0346

ABW: Average Bean Weight; length (L), WB: Width Bean; TB: Thickness Bean; ratio LB/TB.

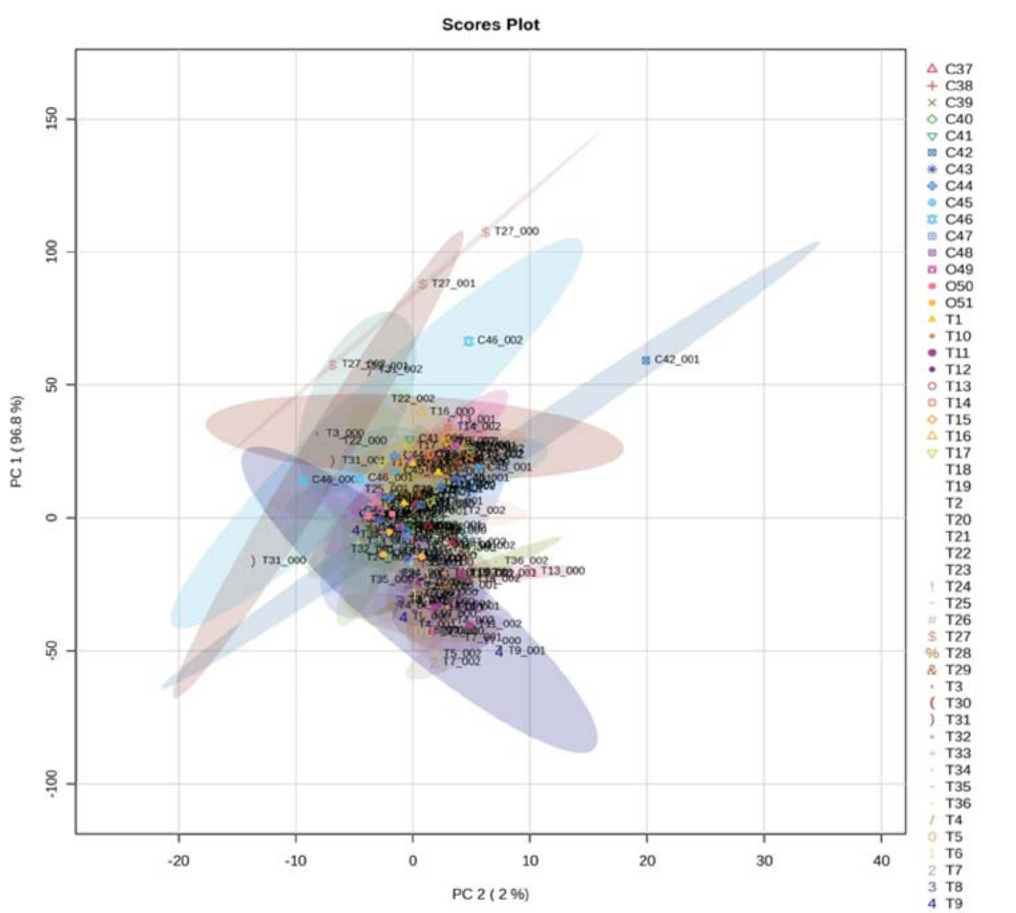

Figure 1. PCA spatial distribution scores for 51 samples of Mexican cocoa beans from different geographical origins (Tabasco=T1-T36; Chiapas=C37-C48; Oaxaca=O49-O51).

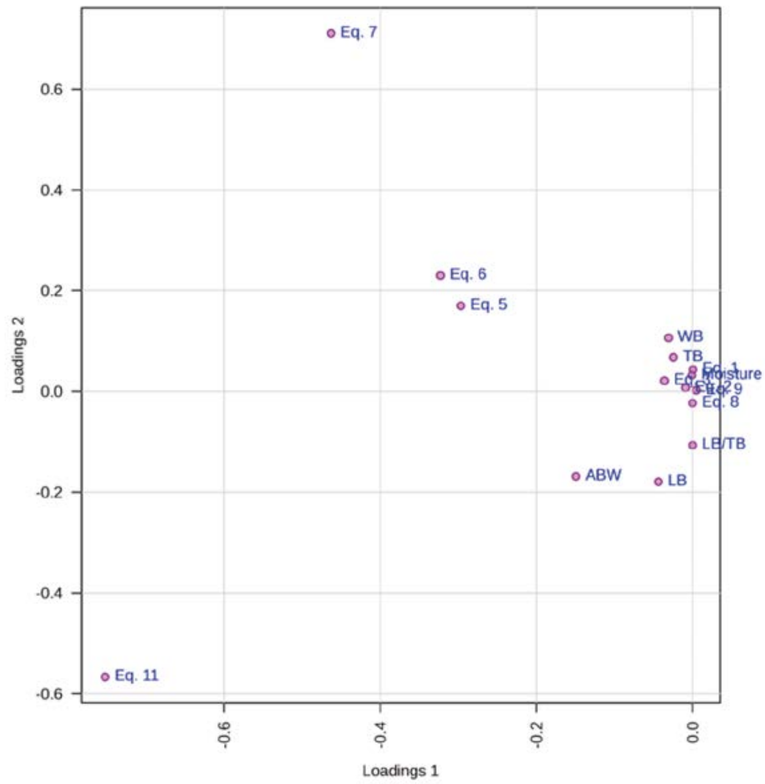

Figure 2. PCA loadings distribution for 51 samples of Mexican cocoa beans from different geographical origins.

groups and crossings is complex due to multiple factors associated with geographical origin, processing (washed and/or fermented cocoa beans), and edaphoclimatic conditions. In their PCA, Oyedokun *et al.* (2011) observed the formation of four groups where the determining factor was bean weight. They also reported that the highest correlation occurred between bean width and thickness, a characteristic feature of the grouping. Likewise, Jaiyeoba *et al.* (2016) observed an inverse relation between moisture and axial dimensions, geometric diameter, sphericity, and surface area. According to Figure 2, the physical parameters that describe the classification are grouped mainly into two domains: the first includes volume (equation 11), bean weight, and bean length, while the second considers equations 5, 6, and 7, corresponding to the expressions of surface area and volume. These results confirm which variables are of more consequence (Table 4).

CONCLUSIONS

Bean weight was the quantitative variable that presented significance. Other measurements, such as length, width, and thickness, were not significant on their own, but they were when combined in the expressions of surface area and volume. Moisture is a critical parameter in dried cocoa beans. However, it did not show significance regarding physical-geometric measurements. The shape factor to describe cocoa beans is an ellipsoid of revolution.

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