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Mathematical modelling of the volumetric contraction of cupuaçu seeds during the drying process

Naeliton de Aquino Gonçalves, Douglas dos Santos Damasceno Gonçalves, Kelder Oliveira Silva, Emilly Aya Mendes Endo, Arlindo Modesto Antunes*, Bruna Sayuri Fujiyama Valente

Department of Agricultural Engineering, Federal Rural University of Amazonia, Brazil

Corresponding author: Arlindo Modesto Antunes ORCID ID: 0000-0001-8652-7249.

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Abstract: Cupuaçu (Theobroma grandiflorum Schum) is a tropical Amazonian fruit that has gained a significant share of the global tropical fruit pulp market. The state of Pará stands out as the largest national producer, with the municipalities of Acará, Tomé-Acu, and Moju being the main production centres. Cupulate®, a product similar to chocolate, is derived from cupuaçu seeds and was developed and patented by Embrapa Amazônia Oriental, located in Pará, in the 1980s. However, the processing of cupuaçu seeds involves several stages, with drying considered the most crucial step as it reduces the moisture content in the seeds, making them less prone to microbiological activity that can lead to spoilage. The aim of this study was to evaluate the volumetric contraction of cupuaçu seeds during the drying process and to fit different mathematical models to the experimental values concerning moisture content. Cupuaçu seeds with an initial average moisture content of 1.5 (decimal d.b.) were used. The seeds were subjected to drying in a prototype vertical fixed-bed drying silo with forced air at temperatures of 55, 65, and 75°C. The volume reduction was analysed as a function of moisture content through different mathematical models fitted to the experimental data, considering the magnitude of error in the estimation of volumetric contraction. The modified Bala and Woods and Polynomial models showed the best fits to the experimental data of apparent volumetric contraction, We recommend that producers employ the Polynomial model to optimise the drying process of cupuaçu seeds at 75°C to achieve improved prod.

Keywords: Theobroma grandiflorum, moisture content, volume, characteristic dimensions.

Introduction

Cupuaçu (*Theobroma grandiflorum* Schum) is an Amazonian fruit that has gained attention in the global tropical pulp market. With a planting area of 8,900 hectares and an annual production of 29,000 tonnes, the state of Pará is the leading producer, with the municipalities of Acará, Tomé-Açu, and Moju standing out. The demand for cupuaçu is driven by the use of its pulp and seeds in the manufacture of various food and pharmaceutical products (Cohen et al., 2005; IBGE, 2023).

The food industry, facing increasing demand, explores cupuaçu seeds, which are rich in fats and proteins. These seeds, with their versatile potential, are used in the production of cupulate, undergoing processes of fermentation, drying, and shell removal. Cupulate, a product similar to chocolate, is obtained from cupuaçu beans and was developed and patented by Embrapa Amazônia Oriental, located in Pará, in the 1980s (Cohen et al., 2005; Braga, 2015).

The cupuaçu tree (*Theobroma grandiflorum* Schum) belongs to the same genus as the cocoa tree (Theobroma cacao L.), whose beans are the raw material for chocolate. Cupuaçu beans undergo several stages similar to those of cocoa until the storage process, such as fruit harvesting, fruit breaking and seed separation, fermentation, drying, and processing of cocoa and cupuaçu beans (Cohen and Jackix, 2005). However, among these stages, drying stands out as the most crucial, as it reduces the water content in the beans, making them resistant to microbiological activity that can result in bean spoilage (Mendes, 2012; Araújo and Silva, 2022).

Knowing the moisture content in agricultural products is extremely important, as it is directly related to the interactions between water molecules and the product constituents. When products have high moisture content, there is an increased risk of infestation by fungi and insects, which compromises seed viability, reduces the vigour of stored grains, and results in significant post-harvest losses (Antunes et al., 2016; Antunes et al., 2017).

The reduction of moisture content involves simultaneous heat and mass transfer processes, which can alter the quality and physical properties of the product, depending on the drying conditions used (Costa et al., 2012). Thus, the loss of water results in damage to the cellular structures of the product, which in turn causes changes in its shape and reduction in its

dimensions (Goneli et al., 2011).

The reduction in product size is a result of the decrease in cellular dimensions due to water loss. This process is known as volumetric contraction (Ramos et al., 2005). When the analysis is performed individually on each grain, we have unit volumetric contraction. On the other hand, when the evaluation is done considering the mass of grains as a whole, we have apparent volumetric contraction (Botelho et al., 2018).

However, it is widely reported that changes in the dimensional characteristics of products during dehydration are considered the main causes of changes in the physical properties of agricultural products (Bala and Woods et al., 1984; Ratti, 1994; Sokhansanj, S., and Lang, 1996). In the specialised literature, there are no records of studies addressing the variation in the size and shape of cupuaçu beans due to the drying process.

Given the above, the present experiment aimed to analyse the effect of moisture content on the apparent volumetric contraction of cupuaçu beans (*Theobroma Grandiflorum* Schum) during the drying process and to fit mathematical models to the experimental data obtained at different temperatures of 55°C, 65°C, and 75°C, as a function of moisture content. Additionally, it aims to contribute to future studies related to the processing and storage of cupuaçu beans.

Results

The evaluation of the Polynomial and Modified Bala and Woods models in representing the volumetric contraction of cupuaçu seeds yielded notable results. The standard error of estimate (SE) and mean relative error (P) for these models were consistently low, indicating a good fit to the experimental data. Specifically, SE values ranged from 0.0000 to 0.0032, underscoring the models' precision in predicting volumetric contraction within the drying conditions studied. The low SE, particularly in the Polynomial model, emphasizes its accuracy, as SE measures the model's error in the same physical unit as the estimated Variable.

Regarding the model adjustments, the results are consistent with those obtained by (Goneli et al., 2011; Goneli et al., 2014) in their study of castor fruit volumetric contraction. In their research, the Modified Bala and Woods and Polynomial models best fit the drying conditions, with R^2 values of 96.46% and 96.59% at 55°C, 95.20% and 91.82% at 65°C, and 98.75% and 98.13% at 75°C, respectively. Additionally, they observed the lowest P and SE magnitudes: P = 0.85%; SE = 0.0009 at 55°C, P = 2.78%; SE = 0.0032 at 65°C, and P = 1.52%; SE = 0.0032 at 75°C for the Modified Bala and Woods model, and P = 0.00%; SE = 0.0000 at all temperatures for the Polynomial model, (Table 1). These findings corroborate the performance of the Polynomial model in the present study, where it consistently displayed high R^2 values and minimal errors across different drying temperatures.

The results presented in Table 2 demonstrate the constants obtained for the Polynomial and Modified Bala and Woods models at three drying temperatures (55° C, 65° C, and 75° C), used to describe the apparent volumetric contraction of cupuaçu seeds. For the Polynomial model, the constant *a* decreased *B* displayedc showed slighta exhibited a substantial reduction from 0.154 at 55° C to 0.002 at 65° C, before increasing to 0.020 at 75° C. Meanwhile, the constant *B* rose considerably from 0.757 at 55° C to 3.651 at 65° C, before reducing slightly to 2.195 at 75° C. The constant *c* was not applicable for this model, (Table 2). These results indicate that both models adjust well to the experimental data, with temperature having a significant impact on the constants involved.

In this study, the Polynomial model demonstrated a satisfactory fit across various drying temperatures, consistently revealing the highest R² values, all above 95.0% for apparent volumetric contraction. This model was particularly effective at 75°C, where it exhibited the best alignment with the experimental data. The mass of the cupuaçu seeds showed a volumetric reduction of 73% at 55°C, 85% at 65°C, and 66% at 75°C, with moisture content ranging from 0.2 to 1.8 (decimal d.b.). These reductions highlight the Polynomial model's capacity to accurately predict volumetric contraction under varying thermal conditions.

The findings align with previous studies on the volumetric contraction of agricultural products during drying, where Polynomial expressions have been widely considered viable. For instance, similar behavior was reported by (Corrêa Filho et al., 2015) in their work with figs and (Botelho et al., 2018) with soybeans. The consistency of the Polynomial model in representing the volumetric contraction of cupuaçu seeds under different drying temperatures reinforces its applicability in modeling the drying behavior of other agricultural products.

The final values of the physical properties of cupuaçu seeds after the drying process at three temperatures (55°C, 65°C, and 75°C) showed significant variations, (Table 3). The initial volume of wet seeds displayed minor variation across temperatures, ranging from 3662 mm³ to 3776 mm³. However, after drying, a marked reduction in seed volume was observed, with the smallest volume recorded at 75°C (2505 mm³), indicating greater volumetric contraction at higher temperatures. This suggests that increasing the temperature accelerates the reduction in seed volume, likely due to greater moisture loss over a shorter drying time.

The bulk densities of the seeds also exhibited notable variations. The initial bulk density was relatively consistent across the temperatures, ranging from 812 kg.m⁻³ to 899 kg.m⁻³. However, the final bulk density showed a significant decrease after drying, with the lowest value observed at 65°C (541 kg.m⁻³). This can be attributed to both volumetric contraction and moisture loss, which reduce the mass of the seeds without a proportionate decrease in total volume, particularly at higher temperatures.

Apparent volumetric contraction, which reflects the reduction in seed volume after drying, showed the greatest variation at 65°C (436 mm³), while the lowest value was recorded at 75°C (385 mm³). This behaviour can be explained by the influence of temperature on the rate of water evaporation, which occurs more rapidly at higher temperatures, resulting in a shorter drying period and, consequently, less total contraction. Additionally, the contraction index, which quantifies the relationship

Temperature °C	Model	Statistical Parameters		
		P (%)	SE (%)	R ² (%)
55°C	Correa et al. (2004)	0.13%	0.0001	91.06%
	Polynomial	0.00%	0.0000	96.46%
	Modified Bala and Woods	0.85%	0.0009	96.59%
	Exponential	0.08%	0.0001	94.84%
	Linear	0.00%	0.0000	95.46%
	Lang and Sokhansanj	0.00%	0.0000	95.46%
65°C	Correa et al. (2004)	0.07%	0.0001	61.68%
	Polynomial	0.00%	0.0000	95.20%
	Modified Bala and Woods	2.78%	0.0032	91.82%
	Exponential	0.06%	0.0001	70.98%
	Linear	0.00%	0.0000	72.21%
	Lang and Sokhansanj	0.00%	0.0000	72.21%
75°C	Correa et al. (2004)	0.59%	0.0001	74.42%
	Polynomial	0.00%	0.0000	98.75%
	Modified Bala and Woods	1.52%	0.0032	98.13%
	Exponential	0.51%	0.0001	84.03%
	Linear	0.00%	0.0000	86.48%
	Lang and Sokhansanj	0.00%	0.0000	86.48%

Table 1. Standard error of estimate (SE), mean relative error (P), coefficient of determination (R²) for the models used to describe apparent volumetric contraction during drying.

Table 2. Constants of the selected models for describing the apparent volumetric contraction of cupuaçu seed.

Model	Constants	55°C	65°C	75°C	
	а	0.669	0.697	0.285	
Polynomial	В	0.073	0.636	0.964	
	С	0.326	0.296	0.315	
Modified Polo and Woods	а	0.154	0.002	0.020	
Moumeu Bala and Woods	В	0.757	3.651	2.195	
	С	-	-	-	

a, B, c - Constants that depend on the product..

Table 3. Final values of the physical properties of cupuaçu seeds evaluated at the three drying temperatures (55, 65, and 75°C) used in the experiment.

Physical properties evaluated	Temperatures		
	55°C	65°C	75°C
Volume of wet seed (mm ³)	3682	3662	3776
Volume of dry seed (mm ³)	2622	3115	2505
Initial bulk density (kg.m ⁻³)	899	812	873
Final bulk density (kg.m ⁻³)	627	541	614
Apparent volumetric contraction (mm ³)	404	436	385
Water loss (g)	223	192	222
Contraction index	0.73	0.85	0.66
a/ao	0.94	0.95	0.91
B/B ₀	0.91	0.91	0.89
c/c ₀	0.82	1.0	0.82

*Dimensions of seeds (a/a0, B/B0, and c/c0), where: a = Length; B = Width; c = Thickness. Source: Authors, 2023.

Model Designation	Model	Equation
Correa et. al. (2004)	$\Psi = 1 / (a + B \exp (U))$	(6)
Polynomial	$\Psi = (a + BU + cU^2)$	(7)
Modified Bala & Woods	$\Psi = 1 - a \{1 - exp[- B (U_0 - U)]\}$	(8)
Exponential	$\Psi = a \exp(BU)$	(9)
Linear	$\Psi = a + BU$	(10)
Lang and Sokhansanj	$\Psi = a + B(U - U_0)$	(11)

 Ψ - Volumetric contraction index (decimal); U - Moisture content (% d.b.); U0 - Initial moisture content (% d.b.); a, B, c - Constants dependent on the product.



Figure 1. Experimental and predicted values from Polynomial models describing the apparent volumetric contraction of cupuaçu seeds (*Theobroma Grandiflorum* Schum) under a temperature of 55°C.

between final and initial volume, was highest at 65°C (0.85), indicating that this temperature caused the greatest seed shrinkage, while the lowest index was observed at 75°C (0.66).

Water loss was another critical factor influencing the final physical properties of the seeds. Drying at 55°C and 75°C resulted in similar water losses (223 g and 222 g, respectively), whereas a slightly lower loss was observed at 65°C (192 g). These data suggest that although higher temperatures promoted greater contraction, the amount of water lost was similar to that at lower temperatures, indicating a complex relationship between drying rate and the physical structure of the seeds.

Finally, the seed dimensions, represented by the ratios between length (a/a_0) , width (B/B_0) , and thickness (c/c_0) , revealed that seed width remained relatively constant across all temperatures, ranging from 0.91 to 0.89. However, length and thickness exhibited greater variation, particularly at 65°C, where thickness (c/c_0) remained unchanged (1.0), indicating that this temperature achieved a balance between water loss and the preservation of seed physical structure. These results highlight how different drying temperatures distinctly influence the physical properties of cupuaçu seeds, which is critical for the development of optimised drying techniques.

Discussion

The results of this study indicate that the Polynomial and Modified Bala and Woods models are highly effective in describing the apparent volumetric contraction of cupuaçu seeds during drying. The low SE and P values observed across different temperatures suggest that these models are well-suited for predicting volumetric changes in agricultural products under drying conditions. The Polynomial model, in particular, showed a robust performance, with high R² values and minimal discrepancies between predicted and observed data.

The performance of these models in this study mirrors the findings of (Goneli et al., 2011) who reported that the Modified (Bala and Woods, 1984) and Polynomial models were the most effective in representing the volumetric contraction of castor fruit under similar drying conditions. Their study found high R² values across different temperatures, with the Polynomial model consistently exhibiting the lowest P and SE values. This similarity underscores the reliability of the Polynomial model in accurately predicting volumetric changes in various agricultural products.

Further, the results of this study are consistent with those of (Oliveira et al., 2013), who observed that volumetric contraction and geometric diameter of soybeans decreased during drying, with these effects being intensified by increasing temperature. The Polynomial model's ability to capture the rapid reduction in moisture content at high temperatures, leading to a smaller shrinkage index, aligns with the findings of Oliveira et al. This behavior is particularly evident at 75 °C, where the model effectively represented the volumetric contraction of cupuaçu seeds.

The high R² values observed in this study for the Polynomial model are indicative of its strength in linear modeling of volumetric contraction. The consistency of these values across different temperatures suggests that the Polynomial model



Figure 2. Experimental and predicted values from Polynomial models describing the apparent volumetric contraction of cupuaçu seeds (*Theobroma Grandiflorum* Schum) under a temperature of 65°C.



Figure 3. Experimental and predicted values from Polynomial models describing the apparent volumetric contraction of cupuaçu seeds (*Theobroma Grandiflorum* Schum) under a temperature of 75°C.

is not only effective but also versatile in its application. This versatility is further highlighted by the model's performance at 75°C, where it provided the most accurate representation of the seeds' volumetric contraction.

In contrast to other models that may require more complex calculations, the simplicity of the Polynomial model makes it a practical choice for modeling volumetric contraction in agricultural products. The model's ability to maintain high accuracy with minimal computational effort is a significant advantage, particularly in large-scale agricultural studies where efficiency is crucial.

The results obtained in this study also corroborate the findings of (Corrêa Filho et al., 2015), who reported similar behavior in the volumetric contraction of figs during drying. Their study highlighted the effectiveness of Polynomial models in capturing the drying dynamics of figs, which is consistent with the results observed in the present study for cupuaçu seeds. This further validates the use of Polynomial models in agricultural drying studies.

Moreover, the study by (IBGE, 2023) on the drying behavior of soybeans also supports the findings of this research. Their work demonstrated that Polynomial models could accurately describe the volumetric contraction of soybeans under different drying conditions, with high R² values and low error margins. The consistency of these results with the findings of the present study reinforces the applicability of Polynomial models in the drying process of various agricultural products. In summary, the Polynomial model has proven to be a reliable tool for predicting the volumetric contraction of cupuaçu seeds during drying. Its high accuracy, simplicity, and consistency with previous studies make it an excellent choice for modeling the drying behavior of agricultural products. The results of this study not only confirm the effectiveness of the Polynomial model but also highlight its potential for broader application in agricultural research.

The findings from this study have practical implications for the drying process of cupuaçu seeds and potentially other agricultural products. The Polynomial model's simplicity and effectiveness make it a strong candidate for further application in the industry, particularly in optimizing drying processes for various seeds.

Future research could explore the application of these models to other seeds or under varying environmental conditions.

Additionally, investigating the long-term impact of different drying temperatures on seed quality could provide valuable insights for agricultural practices.

Materials and methods

Study location

The experiment was conducted at the Rural Engineering Laboratory of the Federal Rural University of the Amazon, Campus Tomé-Açu/PA. The geographical coordinates are 02° 24' 15" S and 48° 09' 51" W (Araújo and Silva, 2022).

The seeds were collected from a cooperative located in the municipality of Tomé-Açu in 2023, fermented for 5 days, with intact and healthy seeds being selected. The region's annual rainfall is 2.300 mm, with an average annual temperature of 26.4°C and an average relative humidity of 85% (Pachêco et al., 2008).

Drying experiment

Sample selection and preparation

Initially, the seeds were cleaned and selected, with all deformed ones being removed. The cupuaçu seeds had an average initial and final moisture content of 1.5 and 0.15 dry basis (decimal d.b.), respectively. The initial and final moisture content of the seed mass was determined using the standard oven method at $105 \pm 1^{\circ}$ C with three repetitions for 24 hours, conducted according to the Rules for Seed Analysis (Brasil, 2009). The dryer used is illustrated in Figure 1, while its operational diagram is shown in Figure 2.

Temperature and drying time

The evaluation of the mass volumetric contraction during drying followed the methodology described by Botelho (Botelho et al., 2018). The reduction in moisture content over the drying time was measured gravimetrically using a prototype vertical fixed-bed drying silo with forced induced air, set at temperatures of 55°C, 65°C, and 75°C.

Three repetitions were performed at each temperature, using 500g of seeds to represent the seed mass, and three repetitions with 10 seeds placed in 1kg micro-perforated plastic nets, considering the initial moisture content of the seeds. An analytical balance with 0.01g precision was used for this measurement.

Specific Mass

To determine the granular specific mass of the seeds, a plastic container with a known volume (0.000527 m³) was used to accommodate the seeds, and the mass of this volume was weighed on an analytical balance with 0.01g resolution (Silva, 2009). The apparent specific mass, expressed in kg.m³, was determined by the seed mass and the volume occupied by them, using three repetitions. Equation 1 was used for the determination:

$$\rho_{ap} = \frac{m}{V}$$

(1)

where:

 ρ_{ap} - apparent or granular specific mass of the product (kg.m⁻³); m - mass of the product (kg); V - volume occupied by the product mass (m³).

Sphericity of the seeds

Data were collected periodically at intervals of 1 hour and 30 minutes, totalling 6 hours, with a total of 5 repetitions throughout the drying process. Both the total mass of the seeds and the set of 10 seeds were removed from the dryer and subjected to measurement of their characteristic dimensions. These dimensions were obtained by determining the seed mass volume and measuring the three orthogonal axes of each seed using a digital caliper.

For cupuaçu seeds, an elongated tri-radial ellipsoid shape (tri-axial prolate ellipsoid) was assumed, as illustrated in Figure 5. According to (Sul-Unijuí and De Vasconcellos, 2012), grains and fruits have geometrically undefined shapes, requiring the adoption of a known shape to solve geometry-related problems, resulting in approximations and possible errors.

However, most agricultural products use geometric shapes of a spheroid or ellipsoid, composed of three characteristic dimensions: the major, intermediate, and minor axes. Methods for determining sphericity, which measures the degree of approximation of the product shape to a sphere, and circularity, which indicates the proximity of the projection area of the material at rest to a circle, were proposed to evaluate these discrepancies, as represented by equation 2 (Agrawal et al., 1972; Mohsenin, 1986).

where:

- a Length in mm;
- b Width in mm;
- c Thickness in mm.
- Unit Volume of the Seeds

To determine the product volume, it was considered a tri-axial prolate ellipsoid with dimensions measured by a digital caliper with 0.1mm resolution. Equation 2 was used to determine the volume, while the volumetric contraction index (Ψ)



Figure 4. Prototype of a vertical fixed-bed drying silo with forced induced air.



Figure 5. Digital caliper. Source: Authors, 2023.



Figure 6. Schematic drawing of a cupuaçu almond, where "a", "b", "c" represent the major, intermediate, and minor characteristic dimensions of the product, respectively.

during drying was determined by the ratio between the volume for each moisture content and the initial volume, as seen in equation 3 (Camicia et al., 2015; Goneli et al., 2011).

 $V = \frac{\pi(abc)}{6}$ (2)

where:

V - Volume at each moisture content, m³;

- a Length in m;
- b Width in m;
- c Thickness in m.

$$\Psi = \frac{V}{V_0}$$

where:

 Ψ - volumetric contraction index, decimal;

V - Volume at each moisture content, m³; and

(3)

V0 - initial volume, m³.

Mathematical Models

The adjustment of mathematical models was performed through non-linear regression analysis using the Gauss-Newton method, with the STATISTICA® software (version 10.0), where the model fit degree was evaluated by the magnitudes of the standard estimation deviation (SE) and the mean relative error (P). Generally, the smaller these indices, the better the model fits the observed data.

Models with mean relative error values less than 10% were considered to have satisfactory fit (Mohapatra and Rao, 2005). The SE and P values for each model were calculated by Equations 4 and 5, respectively:

$$P = \frac{100}{n} \cdot \sum \frac{|Y - Y_0|}{Y}$$
 (4)

$$SE = \sqrt{\frac{\Sigma(Y - Y_0)^2}{GLR}}$$
(5)

Y - observed experimental value;

Y0 - value calculated by the model;

n - number of experimental observations;

GLR - degrees of freedom of the model (number of data minus the number of model parameters).

Besides the mean relative error and standard estimation deviation, the coefficient of determination (R^2) and the trend of residual distribution, which are the differences between experimentally observed and model-estimated values represented as a function of estimated levels, were also considered Botelho (Botelho et al., 2018).

The experimental data of volumetric contraction of the cupuaçu seed mass were fitted to mathematical models traditionally used by various authors, (Koç et al., 2008), (Goneli et al., 2011) castor bean, (Corrêa Filho et al., 2015) fig, (Leite et al., 2015) banana, (Coradi et al., 2016) corn, and others, to describe the volumetric contraction of agricultural products (Meneghetti et al., 2012).

In the mathematical models (Table 4), equations 6 to 11 are adaptations based on moisture content, fitted to the experimental volumetric contraction index (Ψ) data.

Conclusion

The modified Bala and Woods and Polynomial models are the ones that best fit the experimental data of apparent volumetric contraction of cupuaçu almond mass under the drying conditions used. The Polynomial model was chosen for its simplicity. At 75°C, the almond mass exhibited the shortest time to reach the same rate of apparent volumetric contraction, the smallest volume reduction, the lowest shrinkage index, and the best fit of the Polynomial model compared to the other temperatures. The Polynomial model is the most suitable for fitting the experimental data of volumetric contraction of cupuaçu seeds, considering the analyzed conditions.

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Conflicts of Interest

The authors decare no conflicts of interest regarding the publication of this paper.

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