

Kinetics of drying and physical expansion of organic coffee beans during roasting: Mathematical modeling

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ABSTRACT

Coffee roasting is a crucial step in coffee processing, as the beans undergo important chemical and physical transformations that are directly related to the quality of the beverage. Many studies report on kinetics and mathematical modeling of different types of coffee bean drying, but it is necessary to understand the behavior of beans during the roasting process. This study sought to evaluate and model the behavior of the physical properties of organic coffee beans during the roasting process, focusing on volumetric and surface expansion and drying kinetics, in order to propose mathematical expressions applicable to mass and energy balances in the roasting process. The moisture content, water activity, specific mass, and dimensions of the beans were determined at different points during the roasting process. The experimental data were adjusted using mathematical expansion and drying models. The results indicated a progressive reduction in moisture content and in water activity from, contributing to the efficiency of thermal drying and the stability of the final product. In addition, an increase in volumetric and surface expansion was observed, followed by a reduction in the specific mass of the beans. Overall, the models developed and validated ($R^2 > 0.90$, $P < 10\%$, $SE < 1\%$, and residues with random behavior) proved to be effective tools for simulating and predicting the physical transformations that occur during the coffee bean roasting process. These models also help to elucidate the dynamics of the roasting process, enabling their application for optimizing and controlling the coffee roasting process.

Key words: *Coffea arabica*; Campos-Copace model; Nelder-Mead simplex algorithm; Typica variety.

1 INTRODUCTION

Arabica coffee is the most widely grown and consumed coffee species and has the greatest economic importance. This type of bean produces a more refined and smooth beverage, and Brazil has been gaining prominence in the production and export of this product (Freitas et al., 2024; Neves, Cruz & Behrens, 2025). Among Brazilian states, Pernambuco has been reestablishing its coffee production, particularly in the municipality of Taquaritinga do Norte, where smallholder farmers cultivate coffee in intercropping systems with other crops and utilize these organic materials as soil amendments (Santos et al., 2025).

Coffee fruit goes through a long production chain comprising several stages, including planting, harvesting, cleaning, processing, storage, roasting, grinding, packaging, and distribution. Ensuring that all stages are properly aligned is essential to guarantee the quality of the final product. In addition to the inherent characteristics of green coffee beans, roasting is one of the processes that exerts the greatest influence on the color, flavor and aroma of the beans and, consequently on the final quality of the beverage (Bustos-Vanegas et al., 2018; Alcantara et al., 2025).

The roasting subjects coffee beans to high temperatures causing them to undergo significant physical and chemical

modifications, such as the loss of moisture, release of CO₂ and other volatile gases, reduction in the levels of free amino acids, proteins, and sugars (due to Maillard and caramelization reactions, for example), migration of oils to the bean surface, degradation of chlorogenic acids, among others (Wang et al., 2025). Due to the heat and various reactions that occur during roasting, the beans also undergo changes in color, mass, and density, as well as structural changes such as alterations in porosity and volumetric and surface expansion (Al-Shemmeri et al., 2024). Controlling these parameters, as well as the time-temperature combination, is essential to guide the chemical transformations that will determine the sensory characteristics of the final product (Moon et al., 2025).

In this context, mathematical modeling presents itself as a relevant alternative for quality control in the roasting process, as it enables the prediction of the behavior of process variables by simulating these models in scenarios similar to those found in industrial-scale processes (Taite & Dinapoli, 2025). In recent years, several models have been developed based on the physical properties of coffee beans as a control and prediction tool. However, a significant research gap remains due to the fragmentation in the approaches. Some studies focus on the bean drying stage (Araújo et al., 2021; Kumar et al., 2023), while others evaluate the porosity, physical, and thermophysical properties of the beans (Al-Shemmeri et al.,

2024; Bustos-Vanegas et al., 2018). These parameters are critical as they directly influence the heat and mass transfer rates during roasting and determine the development of the bean's internal porosity, which is essential for the retention of aroma compounds and the final quality of the beverage (Bustos-Vanegas et al., 2025).

To address this, the present study differentiates itself by providing an integrated approach that simultaneously evaluates drying kinetics and volumetric and surface expansion, specifically for organic coffee beans. Furthermore, there is a lack of specific models for organic coffee beans, whose distinct structural characteristics, resulting from sustainable cultivation practices, may limit the applicability of models derived from conventional crops. Therefore, the concurrent evaluation of these properties is essential to provide more accurate parameters for the optimization and control of the roasting process.

Thus, this study aimed to evaluate and model the behavior of the physical properties of organic coffee beans (*Coffea arabica*) during roasting, with an emphasis on volumetric and surface expansion and drying kinetics, to propose mathematical expressions applicable to mass and energy balances in the roasting process.

2 MATERIAL AND METHODS

2.1 Obtaining raw materials and the roasting process

The organic coffee beans of the Typica variety, harvested in 2020/2021 and grown at an altitude of 790 m above sea level, were obtained from one of the producers of the Taquaritinga do Norte Organic Producers Association (APROTAC), owner of the Sítio Várzea Grande Farm, located in the city of Taquaritinga do Norte (7°53'54.5"S, 36°2'00.0"W), in the Agreste region of the state of Pernambuco, Brazil.

The roasting process was carried out in a rotary drum roaster, Atila from the Gold Plus 10 kg line (Belo Horizonte, MG, Brazil). To evaluate the physical properties of the beans during roasting, samples were taken during the process and labeled as follows: P0 (raw bean), P1, P2, P3, P4, P5 (intermediate points), and P6 (fully roasted bean) (Figure 1). In addition, the times and temperatures at which each sample was taken are shown in Table 1.

To ensure experimental repeatability and statistical validity, all analyses were performed in triplicate for each sampling point. For each replicate, 10 coffee beans were randomly selected, totaling 30 beans per point, thereby ensuring the representativeness of the treatment and the reliability of the data.

The samples were stored at room temperature (25±2°C) until the analyses were performed: moisture content, using the direct drying method in an oven at 105°C according to the

methodology proposed by the Instituto Adolfo Lutz (2008) and expresses in % dry basis, and grain water activity based on direct reading of the ground sample in a water activity analyzer (Pre Water Activity Analyzer, Aqualab, Pullman, United States).



Figure 1: Sample collection points during the roasting process: A) P0, B) P1, C) P2, D) P3, E) P4, F) P5, G) P6 (n = 3 replicates of 10 beans each per point).

Table 1: Specifications of the time and temperature variables at the sample collection points during the roasting process.

Sample	Time (s)	Temperature (°C)
P0	0	30.00
P1	180	94.50
P2	415	148.00
P3	546	172.65
P4	646	187.35
P5	705	197.40
P6	780	204.90

To determine grain volume, an approximate semi-ellipsoid shape was considered (Mohsenin, 1986) and, using a digital caliper (MTX-316119, China; resolution ± 0.01 mm), the major, intermediate, and minor axes were measured and designated a, b, and c, respectively. The unit volume of the raw grain (P0) (Equation 1) and the other points was determined, and then the volumetric expansion index (Ψ) (Equation 2) was determined for each point. After that, the average volumetric index of the samples for each determined time interval was calculated.

$$V = \frac{abc}{6} \quad (1)$$

$$\Psi = \frac{V_0}{V_f} \quad (2)$$

Where:

a, b, c - grain axis measurements (m);
 V_f - final grain volume in the time interval (m³);
 V_0 - volume of raw grain (m³).

The model cited by Mohsenin (1986) was also used to determine the surface area of the grains (A), finding the unit surface area (Equation 3) of the raw grains (P_0) after each sample was collected. Next, the surface expansion index (ΔS) (Equation 4) and the average surface index for the samples in the time interval were determined.

$$A = \left[\frac{\pi bc + \frac{\pi a \sqrt{2bc}}{2\sqrt{1-\frac{2bc}{a^2}}} \times \sqrt{1-\frac{2bc}{a^2}}}{2} \right] + \frac{\pi ab}{4} \quad (3)$$

$$\Delta S = \frac{A_0}{A_f} \quad (4)$$

Where:

A_f - final grain surface area at the time interval (m^2);

A_0 - surface area of the raw grain (m^2).

The specific mass of the grains was calculated from the previously obtained mass and volume data (Equation 5). The specific unit mass was calculated, in addition to the average specific mass of the grains at each point.

$$\rho = \frac{m}{V} \quad (5)$$

Where:

m - mass of the grain (kg);

V - volume of the grain (m^3).

Mathematical models commonly used to describe grain expansion and contraction processes were used to determine the volumetric expansion index as a function of grain moisture

content (Table 2), as described by Botelho et al. (2018). The model proposed by Bala and Woods (1984) was adapted to meet the specific conditions of this study.

The computational code was developed using GNU Octave software, version 6.2.0, which enabled the mathematical modeling of the experimental data. To initiate the modeling, the code assigns values to the model parameters (Table 2) through a random trial. Based on these values, the volumetric expansion index (Ψ), surface expansion index (ΔS), and moisture ratio (x) are estimated. Subsequently, the code calculates the mean squared error between the experimental values (collected from the ".txt" file) and the values estimated by the model.

To obtain an estimated value as close as possible to the experimental one, a function based on the Nelder–Mead Simplex algorithm, a derivative-free optimization method, was employed to minimize the mean squared error between the values. This optimization algorithm is suitable for functions presenting discontinuities (Quarteroni, Saleri & Gervasio, 2014; Eaton et al., 2021). After obtaining the optimal model parameters, the coefficients of determination (R^2), the relative mean error (P) (Equation 6), and the standard error of estimate (SE) (Equation 7) were calculated to assess model bias and precision. Finally, the code outputs the optimal parameter values (under these conditions) and the associated errors.

$$P = \frac{100}{n} \times \sum_{i=1}^n \frac{|Y_i - \hat{Y}_i|}{Y_i} \quad (6)$$

$$SE = \sqrt{\frac{\sum_{i=1}^n (Y_i - \hat{Y}_i)^2}{GLR}} \quad (7)$$

Where:

Y_i - observed value;

$\hat{Y}_i$ - value estimated by the model;

n - number of observed data;

Table 2: Mathematical models used to model the volumetric expansion of coffee beans.

Models	Equation	References
Corrêa	$\Psi = 1 / (a + b \exp(X))$	Botelho et al. (2018)
Exponential	$\Psi = a \exp(bX)$	Botelho et al. (2018)
Polynomial	$\Psi = 1 + aX + b(X)^2$	Botelho et al. (2018)
Rahman	$\Psi = 1 + a(X - X_0)$	Rahman (1995)
Bala and Woods	$\Psi = 1 - a\{1 - \exp[-b(X - X_0)]\}$	Bala and Woods (1984)
Copace (2014)	$\Psi = 1 / [1 + a(X_0 - X) + b(X_0 - X)^2]$	Bustos-Vanegas et al. (2018)
Campos-Copace	$\Psi = a(X_0 - X)^3 + b(X_0 - X)^2 + c(X_0 - X) + d$	Bustos-Vanegas et al. (2018)

Ψ - unit volumetric expansion index (dimensionless); X_0 - initial grain moisture content (decimal dry basis); X - grain moisture content at time t (decimal dry basis); a , b , c = model parameters.

GLR - Degrees of freedom of the residual (characterized by the number of observed data minus the number of model parameters).

3 RESULTS

3.1 Kinetics of the physical parameters of coffee beans

When measuring the moisture content during the coffee roasting process, a gradual decrease in this parameter is observed, with a reduction of approximately 76.89% between P0 and P6 (Figure 2A).

Regarding water activity (A_w), a behavior similar to that of water content was observed, with a continuous decrease

throughout the process, corresponding to a percentage reduction of approximately 35.48% between the start and end of the roasting process (Figure 2B). When evaluating the volumetric expansion index (Ψ), the coffee beans exhibited an increase in volume throughout almost the entire roasting process with a gradual increase starting from P1 ($\Psi = 0.99 \pm 0.07$) (Figure 2C). The beans reached a maximum Ψ of 1.53 ± 0.16 at the end of roasting (P6), corresponding to a 53% increase in their volume (Figure 2C).

In general, it can be seen that the greatest expansions occurred between points P1 (94.5 °C), P2 (148.0°C), and P3 (172.65°C), which can be explained by the reactions that occur in this temperature range.

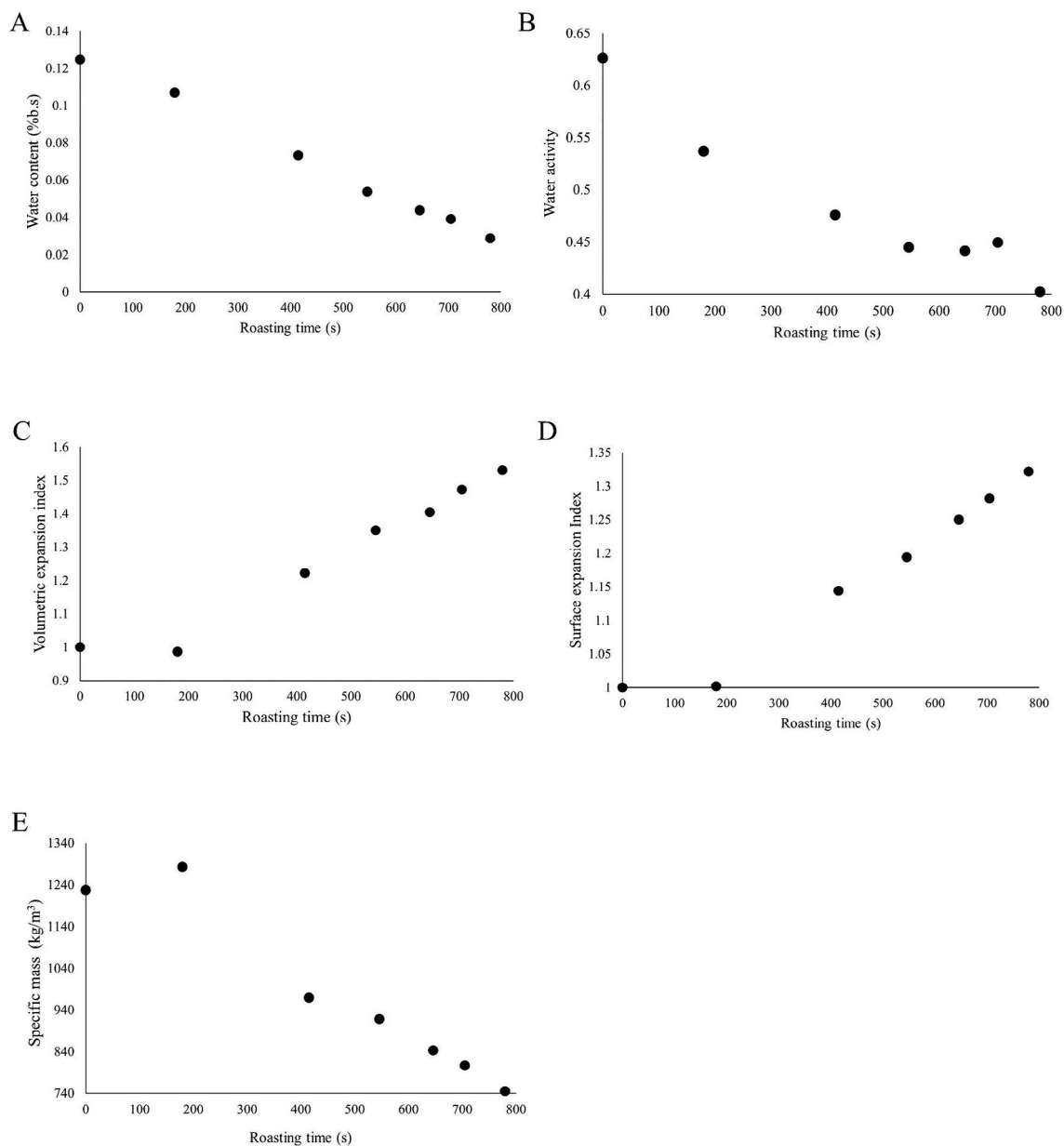


Figure 2: Kinetics of physical parameters evaluated in coffee beans during the roasting process: (A) Moisture content (% dry basis), (B) Water activity (A_w), (C) Volumetric expansion index, (D) Surface expansion index, (E) Specific mass (kg/m³).

The greatest variation in grain surface area was observed between points P1 and P2, where the surface expansion index increased by approximately 11.76% (Figure 2D). At the end of the roasting process, sample P6 exhibited a maximum expansion index of 1.32 ± 0.07 , corresponding to an approximate 32.1% increase in the surface area of the beans (Figure 2D).

Regarding specific mass, the green coffee beans (P0) started the roasting process with a specific mass of $1227.98 \pm 41.80 \text{ kg/m}^3$. At point P1, a slight increase in this parameter was observed, which may be related to volumetric contraction (Figure 2E). Afterward, the specific mass decreased until the end of the process, reaching a value of $745.21 \pm 17.63 \text{ kg/m}^3$ (P6), representing an approximate reduction of 39.32%.

The moisture ratio (Figure 3) reflects the dehydration stages of the roasting process. While water vaporization is the primary factor in mass reduction during the early and intermediate phases, the total weight loss observed in the later stages (P4–P6) also incorporates the release of non-water volatiles and products of pyrolysis. Thus, the measured mass loss reflects a combination of moisture removal and the chemical transformations inherent to the roasting degrees evaluated

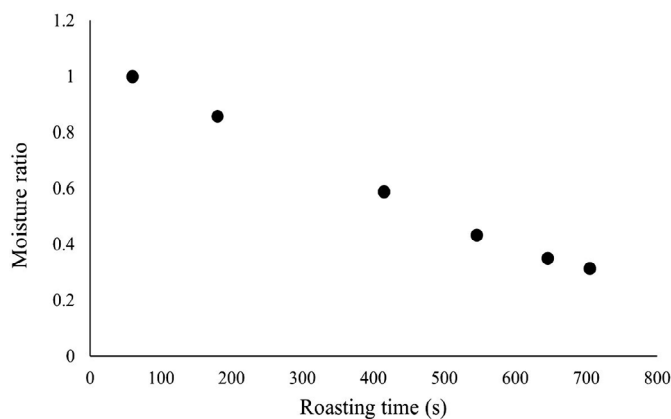


Figure 3: Moisture ratio of coffee beans during the roasting process.

3.2 Mathematical modeling of volumetric and surface expansion

The information on models applied for the study of volumetric and surface expansion, including the estimated parameters (a, b, and c), associated errors (relative mean error and standard error of estimate), and the coefficient of determination (R^2), is presented in Table 3. Although the behaviors of volumetric and surface expansion are similar and can be described by the same mathematical model (Bustos-Vanegas et al., 2018), the models were applied separately to evaluate both parameters, enabling more detailed observation of the expansion processes.

Thus, these residues were distributed according to the Campos-Copace model (Figure 4B and 4D), which

showed random behavior, with no formation of figures and no underestimation or overestimation of values, given that all residues are very close to the horizontal zero line represented by the red line. Therefore, the Campos-Copace model can be used to describe the volumetric and surface expansion behavior of coffee beans during the roasting process and can be described by Equations 8 and 9, respectively.

$$\Psi = -922,5(X_0 - X)^3 + 171,6417(X_0 - X)^2 - 2,5246(X_0 - X) + 1 \quad (8)$$

$$\Delta S = -335,0705(X_0 - X)^3 + 70,184(X_0 - X)^2 - 0,3246(X_0 - X) + 1 \quad (9)$$

4 DISCUSSION

4.1 Kinetics of the physical parameters of coffee beans

This downward trend is associated with the vaporization of moisture contained in the beans, a phenomenon characteristic of the initial drying stage of roasting (Al-Shemmeri et al., 2024). This significant water loss in the early stages confirms the occurrence of the endothermic phase, in which the energy supplied is mainly used for the evaporation of free water (Schenker & Rothgeb, 2017).

Moisture analysis allows the total water content in a food product to be determined, showing both the free surface water content and the adsorbed water, which is bound. This parameter is essential to ensure the chemical and microbiological stability of grains during storage, since values above the permitted level (approximately 15% dry basis) can allow the development of microorganisms such as fungi, bacteria, and undesirable enzymes, which consequently, increases the risk of contamination by mycotoxins such as ochratoxin A (Lozano, Monje & Guzman, 2025).

The behavior observed of A_w can be explained by the fact that when the grains are heated, the free water inside them initially vaporizes, followed by the bound water, as also observed by Barbosa et al. (2025). In addition, the reduction in A_w indicates a decrease in the availability of free water for chemical reactions and microbial growth, thereby contributing to the stability of the product after the roasting process (Rennert & Hiller, 2023; Barbosa et al., 2025).

When observing the grains, it was noted that they exhibit expansive behavior caused by the production and accumulation of gases such as water vapor, carbon monoxide (CO), carbon dioxide (CO₂), and other volatile compounds generated during the reactions (Alcantara et al., 2025). It is known that, starting at a temperature of 50°C in the roasting process, the first changes

Table 3: Parameters (a, b, and c) estimated by the tested mathematical models for the volumetric expansion index (VEI) and surface expansion index (SEI), along with their respective relative mean errors (P), standard errors of estimate (SE), and coefficients of determination (R^2).

Variable	Mathematical model	Model parameters			Errors		R^2
		a	b	c	P	SE	
VEI	Exponential	-3.2219	3.7606	-	1.8838	0.0312	0.9880
SEI		-1.8812	2.5655	-	1.1652	0.0183	0.9832
VEI	Linear	1.7608	-4.9413	-	1.8623	0.0338	0.9799
SEI		1.4357	-3.1242	-	1.2750	0.0202	0.9794
VEI	Polynomial	4.7124	0.0724	-	4.7124	0.0724	0.8996
SEI		0.2931	-21.7829	-	2.8493	0.0420	0.9037
VEI	Rahman	-5.1533	-	-	2.7873	0,0508	0.9263
SEI		-3.103900	-	-	1.6709	0.0276	0.9398
VEI	Bala e Woods	-107.960	0.0000477	-	2.7874	0.0556	0.9263
SEI		-69.088	0.000045	-	1.6709	0.0303	0.9398
VEI	Copace (2014)	-3.0477	-6.8028	-	1.7422	0.0363	0.9739
SEI		-1.7361	-8.8879	-	0.9760	0.0179	0.9825
VEI	Campos-Copace	-922.50	171.6417	-2,5246	1.0062	0.0209	0.9938
SEI		-335.0705	70.184	-0,3246	0.7944	0.0153	0.9904

(-) Not applicable.

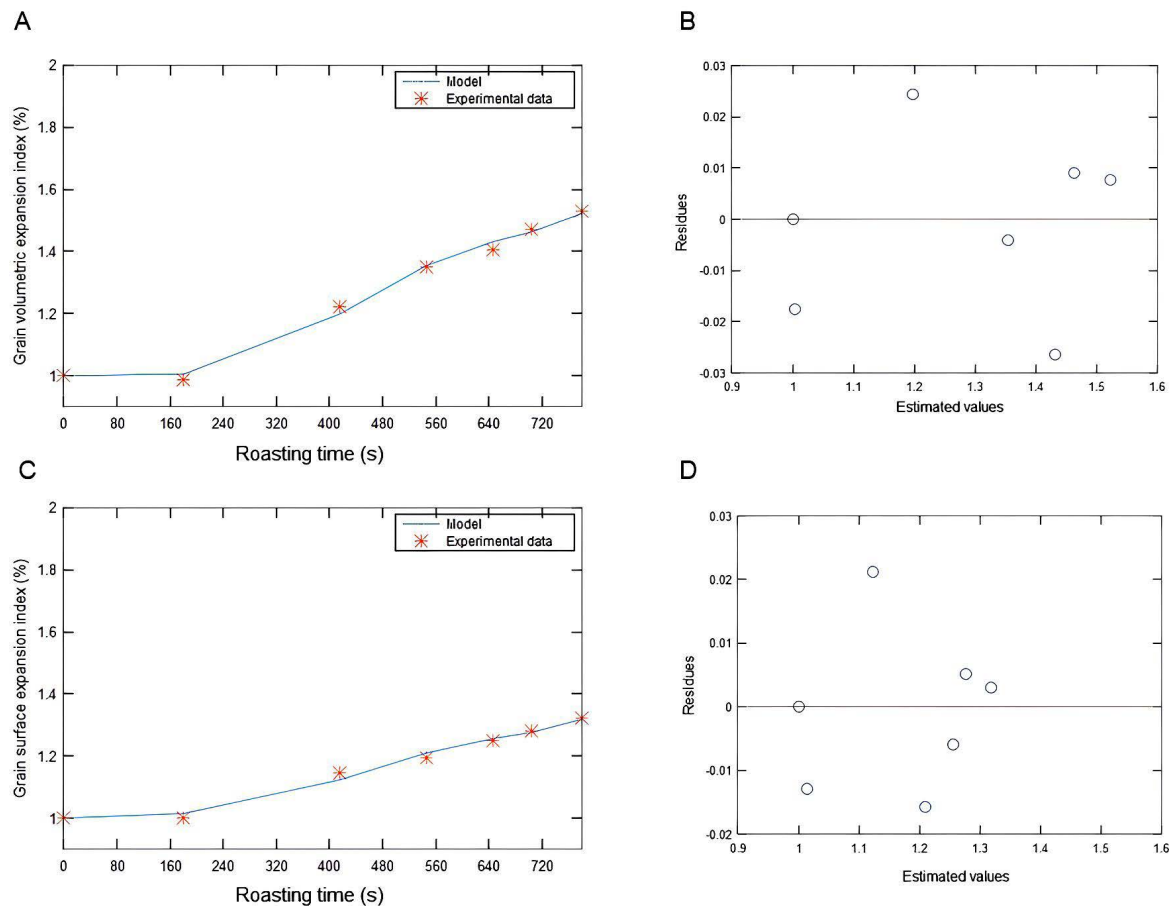


Figure 4: Behavior of the volumetric (A) and surface (C) expansion indices of the beans during the roasting process, using the Campos-Copace mathematical model, and the residues for models (B and D), respectively.

occur in the grain tissue layers, resulting from water evaporation and protein denaturation. When the temperature exceeds 100 °C, the thermal decomposition of the organic part of the grain begins, indicated by the onset of pyrolysis symptoms of the grain as a result of slow combustion. At around 150 °C, gases such as CO₂, CO, and water vapor develop inside the bean, increasing the internal pressure and, consequently, this process causes the tough cellulose-based structure of the green bean to transition from a rigid state to a flexible, rubbery state before finally becoming brittle and rupturing, resulting in expansion a stage known as the “first crack,” usually observed between 180°C and 200°C (Sienald et al., 2024).

With regard to the surface expansion index, the observed behavior was expected, since higher temperatures, such as those reached at point P6 (204.9 °C), cause an increase in volume and surface area, as demonstrated by Bustos-Venegas et al. (2018). On the other hand, the result for specific mass is within expectations, considering that, according to Sienald et al. (2024), roasted coffee beans can show a reduction of up to 56% in specific mass. This decrease in the parameter can be explained by the fact that specific mass represents the ratio between the grain's mass and its volume. As observed throughout the roasting process, due to the changes caused by heat and pressure, the beans swell and expand, along with a reduction in their mass, which results in a decrease in specific mass (Al-Shemmeri et al., 2024).

The correlation between moisture content and mass loss observed in this study is consistent with the findings of Bustos-Vanegas et al. (2018), who proposed linear equations for mass loss prediction across various temperatures. However, our results suggest that this linear relationship is most accurate during the dehydration phase. As roasting progresses to higher degrees (P4–P6), the thermal degradation of organic compounds, such as carbohydrates and proteins, triggers the release of and other non-water volatiles (Schenker & Rothgeb, 2017). This indicates that in darker roasts, the final mass reduction is a combined result of both intense dehydration and the loss of dry matter through thermal decomposition.

4.2 Mathematical modeling of volumetric and surface expansion

The relative mean error was also evaluated, considering that a mathematical model can describe the process if the value of this error is below 10% (Andrade et al., 2019), and for the standard deviation of the estimate, models with SE < 1% were considered acceptable (Botelho et al., 2018).

To fit the model to the data, it is also necessary to observe the behavior of the residuals. According to Botelho et al. (2018), a mathematical model can exhibit either a random or biased distribution of residuals (the difference between the value estimated by the model and the actual value of the variable). A

model with a biased residual distribution shows patterns such as geometric shapes or consistent underestimation/overestimation of the variable. Conversely, a random residual distribution does not present geometric patterns, and the residuals remain close to a constant horizontal line at zero (Figure 4B and 4D).

In this way, it is possible to observe the behavior of the parameters studied throughout coffee roasting. Based on physical characterization and adjustments to the mathematical models, it was observed that structural changes in the beans, such as volumetric and surface expansion, can be represented using moisture-dependent functions by the Campos-Copace model. Thus, physical characterization and mathematical modeling can be applied to understand, predict, and optimize the critical steps of the roasting process in the coffee industry.

The models that best fit the data were the Exponential and Campos-Copace models (Table 3), with coefficients of determination of 0.9880 and 0.9938, respectively. Almost all the models tested are suitable for describing the volumetric and surface expansion of the grains, except for the polynomial model for volumetric expansion index (0.8996).

However, when evaluating all these parameters together and aiming for a more precise fit, the Campos-Copace model proved to be the most suitable to describe the volumetric and surface expansion phenomena of the beans. The models demonstrated that 99.38% and 99.04% (R²) of the variations around the means can be explained by the regression. Moreover, they presented the lowest values for both the relative mean error (P = 1.0062 and 0.7944) and the standard error of estimate (SE = 0.0209 and 0.00153) for the volumetric (Figure 4A) and surface (Figure 4C) expansion behaviors, respectively. Observing the volumetric expansion indices estimated by the model (Figure 4A), it is noted that they were close to the experimental indices, which explains why the curve exhibited a coefficient of determination so close to 1.

Studies evolving the reactions that occur in the coffee roasting process need to be understood in depth, considering all the variables that can influence the process. Thorough knowledge of these phenomena will help in producing a coffee with high nutritional and sensory quality, as well as the optimization and equipment planning, in addition to reducing operating and experimental costs (Bustos-Vanegas et al., 2025).

Finally, this study has limitations that should be considered. The analysis focused on a single origin and cultivar, which may not represent the full diversity of coffee profiles. Additionally, a single roasting profile was used, and the lack of chemical and sensory correlation limits the generalization of the findings. Therefore, future research should include different varieties and roasting degrees to validate and expand these results, as well as to understand consumer sensory perception and acceptance.

5 CONCLUSIONS

Based on the studied parameters, mathematical models accurately described the volumetric and surface expansion of coffee beans. The Campos-Copace model presented the best fit, making it most suitable for this purpose. Thus, under the experimental conditions of this study, the models developed showed potential as tools for simulating and predicting physical transformations during roasting. These findings may contribute to a better understanding of process control, although further validation with cultivars and roasting profiles is necessary to broaden their industrial application.

6 AUTHORS' CONTRIBUTION

Conceptual idea: Medeiros, A.L.T.; Silva, S.P.; Methodology design: Medeiros, A.L.T.; Santos, W.W.V.; Camelo, M.C.S.; Data collection: Medeiros, A.L.T.; Santos, W.W.V.; Silva, G.H.D.S.; Barbosa, P.T.; Data analysis and interpretation: Medeiros, A.L.T.; Santos, W.W.V.; Silva, W.B.; Barbosa, P.T.; Silva, G.H.D.S., and Writing and editing: Medeiros, A.L.T.; Santos, W.W.V.; Silva, W.B.; Barbosa, P.T.; Camelo, M.C.S.; Silva, S.P.

7 DATA AVAILABILITY STATEMENT

Data available upon request to authors.

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