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Evaluation of the behavior of coffee stored in cooled and natural environments

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ABSTRACT

The market value of coffee is strongly influenced by loss of quality, which makes storage one of the main steps in the entire production chain. The finite element method (FEM) and computational fluid dynamics (CFD) are numerical and computational techniques that facilitate the simulation of agricultural product storage systems. Computational modeling satisfactorily represents real experimentation, simplifies decision-making, and reduces costs. This study aimed to analyze mocha coffee storage for 6 months in a cooled environment with temperatures between 15 and 18 °C and in a natural environment. The water content, bulk density, specific heat, thermal conductivity, and thermal diffusivity were determined and colorimetry and sensory analysis were applied to compare initial and final samples of the product after storage. It was found that the water content and specific heat were the only properties that presented significant changes. Through sensory analysis, it was observed that the quality of the coffee was the same for both systems. A computational model was developed to simulate the heat transfer process during storage. The comparison of the simulation results with the experimental results for the temperature distribution in the grain mass showed overall mean relative errors of 2.34% for the natural environment and 5.74% for the cooled environment.

Key words: Coffee; postharvest; storage.

1 INTRODUCTION

The storage of agricultural products allows, among other factors, their distribution and consistent supplies to different markets (Penson et al., 2019). This is an important step in terms of preserving coffee quality before its commercialization. Storage may be accompanied by loss of quality due to quantitative and qualitative changes in the substances present in the grains, which makes the preservation of product quality directly dependent on good storage conditions (Tripetch; Borompichaichartkul, 2019). The main factors that can lead to loss of quality during the storage period are variations in temperature and relative humidity and exposure to light (Borém et al., 2019).

The cooling of the air in storage is a technique for controlling the ambient temperature conditions and consequently the relative air humidity, which are important factors controlling the deterioration process in agricultural products. Reducing the temperature of stored products below 15 °C has been efficient in minimizing water activity and consequently the activity of fungi and pests (Rosa et al., 2013).

Regarding the maintenance of coffee quality, storage in a cooled environment has already been studied in terms of sensory analysis (Borém et al., 2008; Donovan; Foster; Salinas, 2019) and the analysis of chemical and physiological aspects (Pazmiño-Arteaga et al., 2022; Rosa et al., 2013).

The main internal factors that influence the heat transfer process are the production of heat, moisture, and CO_2 due to the respiration of grains, insects, mites, fungi, bacteria, and the physical properties of the stored product (Panigrahi et al., 2020). For heat transfer analyses, the thermal properties of the product, such as the specific heat, thermal conductivity, and thermal diffusivity, are of great relevance (Borém et al., 2002).

The thermal conductivity of a material quantifies its ability to conduct thermal energy. The values of thermal conductivity for solid, granular, and porous materials may vary according to their chemical composition, fluid material content, physical structure, state, density, temperature, and water content. For biological materials, such as grains, the thermal conductivity depends more on the cell structure, density, and water content than on the temperature (Mohsenin, 1980).

The thermal diffusivity represents the heat transfer rate due to the temperature gradient between the hot and cold parts inside a product and between its surface and the external environment. It can be determined from the specific heat, thermal conductivity, and bulk density (Cardoso et al., 2018).

One of the main factors used to classify the quality of coffees is descriptive sensory analysis, in which tasters assign scores to each sensory attribute. Of the methods of sensory analysis, the main method is proposed by the *Specialty Coffee Association* (SCA) (Specialty Coffee Association - SCA, 2008).

Computational fluid dynamics (CFD) is a method for the systematic analysis of heat transfer, mass transfer, and hydrodynamics, among others, through numerical simulation (Ajani; Zhu; Sun, 2020). The finite element method (FEM) is a numerical procedure to determine approximate solutions for differential equation problems with boundary conditions. It has been developed and widely used due to its high reliability and the accuracy of the results (Sabat; Kundu, 2021).

Thus, this study aimed to determine the physical and thermal properties of stored coffee and to simulate the heat transfer process during coffee storage under different conditions for comparison to meet the demands of specialty coffee and commodity storage companies.

2 MATERIAL AND METHODS

The project took place at the Laboratory of Agricultural Product Processing (LPPA, for its abbreviation in Portuguese) of the Federal University of Lavras (UFLA) and at a company in the municipality of Varginha, in the southern region of Minas Gerais, Brazil. The raw material used in the experiment was a commercial lot containing different varieties of hulled mocha grains. The product was stored at the company, and the analyses were performed in the LPPA.

The coffee was stored in jute sacks for 6 months from November 2019 to May 2020 in conventional storage and conventional storage in a cooled environment (15 to 18 °C). The physical properties were determined for the initial coffee samples, which were the same for both storage methods, and for the final coffee samples – only for the coffee stored in a cooled environment. These samples were referred only as the initial and final samples, respectively.

In both storage systems, the piles of coffee sacks had the same physical composition. The ballast used for the sack distribution was 10 sacks. Each ballast represents a distribution of sacks in a vertical layer. The ballast in the layer above or below was always rotated by 180°, which allowed the mooring of the pile. Each pile contained 7 layers, thus adding a total of 70 sacks in each of the environments.

Figure 1 illustrates the ballast used in the composition of the piles and the configuration of the ballast in two consecutive layers.

The product Cocoon Lite 005, manufactured by the company GrainPro, was used for storage in a cooled environment to properly isolate the coffee beans. Cocoon is a polyethylene wrap that minimizes gas and water exchanges with the external environment. This product is not intended for thermal insulation; however, it was used due to the practicality of adaptation to the experiment, as well as to verify its efficacy for storage of cooled coffee through scientific experimentation.

A cooler for grains and seeds was used to maintain low temperatures inside the cocoon. This cooler is not a commercial model and is used only for research. The equipment was programmed to turn on the cooling system when the grain mass reached 18 °C and to turn off when it reached 15 °C to keep the product in the desired temperature range.

A probe was used to monitor the temperature of the grain mass under the regulation of the control panel of the cooling equipment. This probe passed through one of the air outlets of the cocoon and was positioned in contact with the coffee beans in one of the sacks at a distance approximately 0.5 m inside the pile. Figure 2 shows the positioning of the probe.

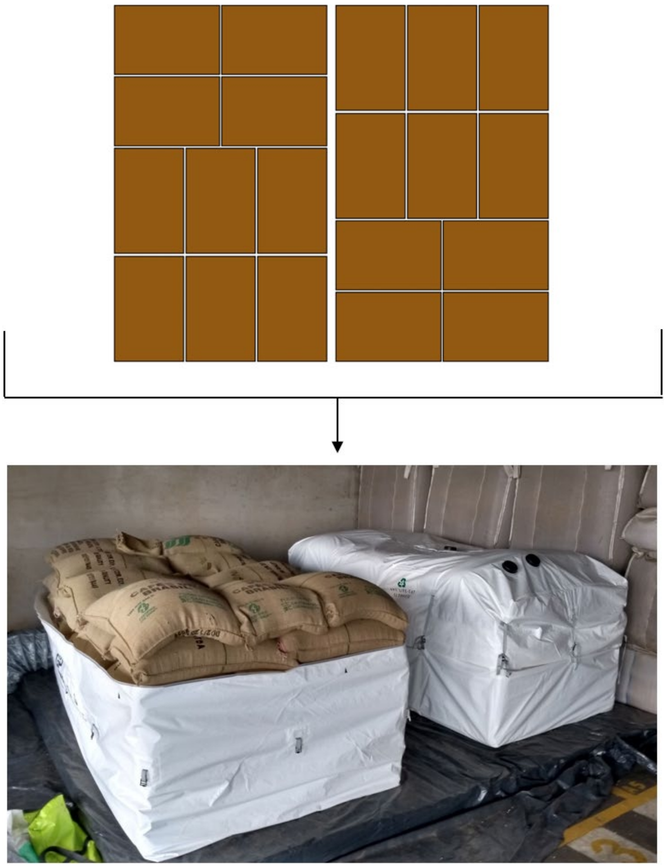

Figure 1: Schematic of the ballast used in the piles during storage and the positioning in two consecutive layers.
Source: Authors (2022).

Figure 2: Probe positioned through an air outlet of the cocoon, measuring the grain mass at approximately 0.5 m below the top of the pile.
Source: Authors (2022).

A total of 22 identical sensors were used to monitor the temperature of the grain mass during storage. There were 15 sensors in the cooled environment and 7 in the natural environment. Fewer sensors were used in the natural environment because the temperature oscillation of the pile in this environment was much smaller since it followed the ambient temperature and stabilized. Each of the sensors was identified with a corresponding number, and their position was recorded. At the end of the storage period, the temperature data from the sensors were compared to those obtained by process simulation, and the comparison showed that the model was a faithful representation of the system.

The physical properties of the initial and final coffee samples were determined in the LPPA of UFLA. These properties included the water content, bulk density, and color parameters.

The water content of the samples was determined by the ISO 6673:2003 standard method (International Organization for Standardization - ISO, 2003), which consists of placing the samples in an oven at 105 ± 1 °C for 16 ± 0.5 hours.

The bulk density of the beans was determined by using a Gehaka kit to determine their hectoliter weight and then converting the hectoliter weight to $kg.m^{-3}$. Three replicates were performed for each sample (initial and final).

Colorimetry measures color by means of objective measurements. A colorimeter is a device that separates the red, green, blue (RGB) light components, providing colorimetric coordinates ($L^*a^*b^*$) that can be reproduced with great accuracy. In this system, "L" indicates lightness (0 = black and 100 = white) and "a" and "b" indicate the representation of opponent colors: +"a" = red, -"a" = green, +"b" = yellow, and -"b" = blue (Abreu et al., 2013).

The color of the stored coffee was analyzed using a Minolta CR-300 colorimeter at the beginning of storage and after completion – 6 months later – to assess whether there were significant changes in its color and whether these changes accompanied other changes in product quality.

For the measurements, the samples were placed in Petri dishes, and for each replicate, five readings were performed, one at the central point of the plate and one at each cardinal point, to obtain the mean value for each colorimetric coordinate. Three replicates were performed for each sample.

The changes in color were evaluated by the total color difference (ΔE) between the initial and final samples, obtained by Equation 1.

$$\Delta E = \sqrt{(\Delta L)^2 + (\Delta a)^2 + (\Delta b)^2} \quad (1)$$

Where ΔE is the total color difference between two samples, ΔL is the difference in the L parameters of two samples, Δa is the difference in the parameter a values of two samples, and Δb is the difference in the parameter b values of two samples.

The thermal properties of the initial and final coffee samples were determined in theLPPA of UFLA, namely, the specific heat, thermal conductivity, and thermal diffusivity, according to Cardoso et al. (2018).

The specific heat was determined by the method of mixture. In this method, a product (coffee beans) with a known mass (100 g) and temperature is placed in a calorimeter of known thermal capacity (0.048 $kJ.°C^{-1}$) containing water with a known mass (0.4 kg) and temperature. When the thermal equilibrium of the mixture is reached, the specific heat of the grains can be obtained through Equation 2.

$$C_p \cdot M_p \cdot (T_e - T_p) = C_w \cdot M_w \cdot (T_w - T_e) + C \cdot (T_w - T_e) \quad (2)$$

Where C_p is the specific heat of the product ($kJ.kg^{-1}.°C^{-1}$); C_w is the specific heat of the water ($kJ.kg^{-1}.°C^{-1}$); C is the thermal capacity of the calorimeter ($kJ.°C^{-1}$); M_p is the mass of the product (kg); M_w is the mass of water (kg); T_p is the initial temperature of the product (°C); T_w is the initial water temperature (°C); and T_e is the equilibrium temperature (°C). Figure 3 shows a diagram of the method used to determine the specific heat.

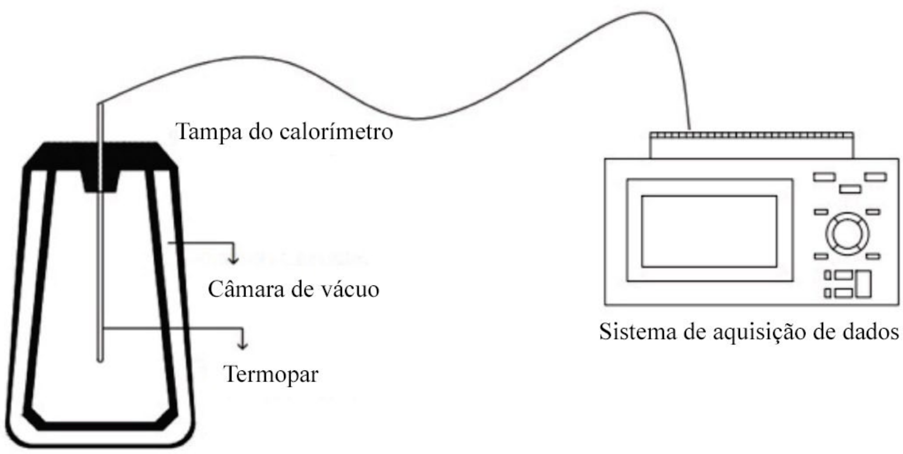

Figure 3: Schematic representation of the specific heat determination.

Source: Adapted from Cardoso et al. (2018).

Three replicates were performed for each sample (initial and final). The thermal conductivity was determined by using the infinite cylinder method. This method consists of placing a grain sample in an aluminum cylinder with known diameter and length, with a varnished nickel-chromium resistor wire along the central axis, through which a low-intensity electric current passes (approximately 1 A). The temperature inside the grain mass was obtained by means of thermocouples positioned at half the height of the cylinder. Figure 4 shows a schematic representation of the system used to determine the thermal conductivity.

For each of the three replicates, the cylinder with coffee was kept in a biochemical oxygen demand (BOD) incubator with a constant temperature of 20 °C for 12 hours for temperature stabilization, without the passage of electric current through the resistor wire. After this period, the source that produces the current was turned on, and temperature data from inside the grain mass were collected every 5 seconds over 6 hours.

The thermal conductivity of the grain mass was obtained using Equation 3.

$$k = \frac{Q}{4 \cdot \pi \cdot (T_2 - T_1)} \cdot \ln\left(\frac{t_2 - t_0}{t_1 - t_0}\right) \quad (3)$$

Where k is the thermal conductivity ($Wm^{-1}.°C^{-1}$); *Q* is the heat generated by the conducting wire (W); t is time (s); T_t is the temperature at time t (°C); and t_0 is the correction factor (s).

The correction factor t_0 can be calculated as a logarithmic function of the time values and the differences between the temperatures observed over time and the initial temperature of the system (Chang, 1986).

The thermal diffusivity of the grain mass was determined from the experimental values obtained for specific heat, thermal conductivity, and bulk density using Equation 4.

$$\alpha = \frac{k}{\rho \cdot C_p} \quad (4)$$

Where α is the thermal diffusivity ($m^2.s^{-1}$); k is the thermal conductivity ($W.m^{-1}.°C^{-1}$); ρ is the bulk density ($kg.m^{-3}$); and C_p is the specific heat of the product ($kJ.kg^{-1}.°C^{-1}$).

The sensory analysis was performed on the initial samples and samples at the end of the 6-month storage period. It was performed by judges certified by the SCA using the SCA sensory evaluation method at the LPPA at the UFLA.

Thus, whether there were changes in coffee quality from the beginning of storage to after storage and whether there were differences between storage in the natural environment and in the cooled environment were evaluated.

The finite element analysis software ANSYS *Workbench* version 20.1 (student) was used to simulate the behavior of the storage systems. It uses the CFD method from the model obtained by the FEM to obtain the behavior of systems involving heat transfer. The simulated systems were those with the cooled environment and the natural environment. For the validation of the model, the numerical simulation data were compared to the results found experimentally, which validated the developed model and evaluated the reliability in the representation of the real storage system.

The mean relative error (Equation 5) was used to evaluate the quality of the models in representing the real systems at each temperature collection point, in both the cooled and natural environments.

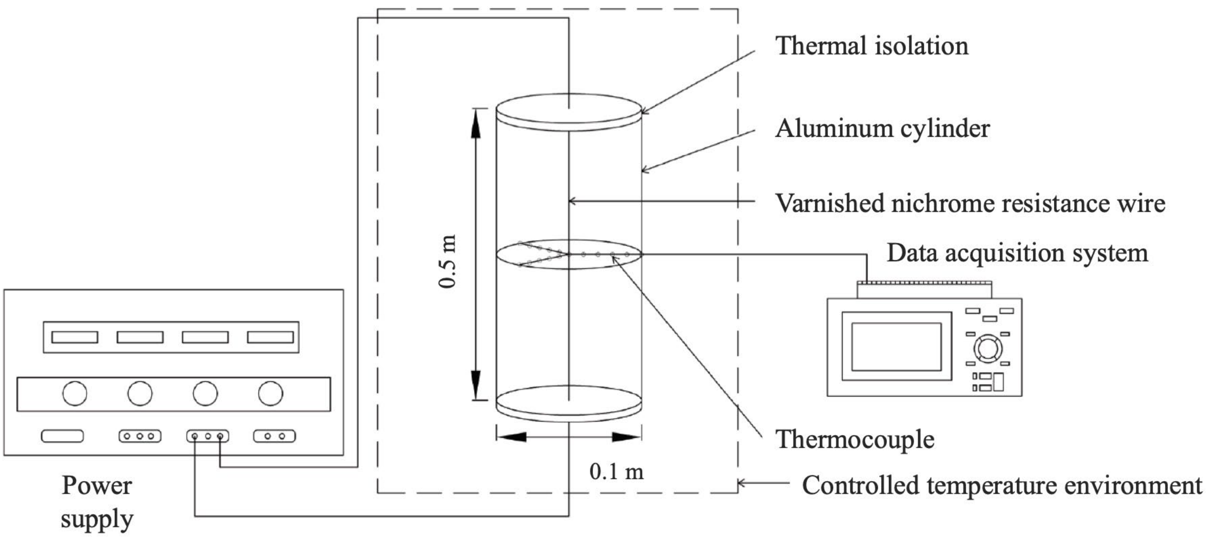

Figure 4: Scheme used to determine the thermal conductivity.
Source: Adapted from Cardoso et al. (2018).

$$P = \frac{100}{n} \cdot \sum \frac{\left|Y - \hat{Y}\right|}{Y} \quad (5)$$

Where P is the mean relative error (%); $\hat{Y}$ is the number of observations; Y is the experimental value observed at a given point; and is the value obtained by the model at the same point.

The overall mean of these errors was then calculated for each storage system.

3 RESULTS

Note that Tukey's test was not applied to the thermal diffusivity because this property was obtained from the results of other properties and there were no repetitions in its determination, which precluded statistical differentiation analysis.

Table 1: shows the physical and thermal properties obtained experimentally for the initial and final samples. A comparison between the values obtained experimentally was performed by using Tukey's test (Tukey, 1953).

Property	Initial sample	Final sample
Water content (% w.b.)	10.08 a	10.67 b
Bulk density ($kg.m^{-3}$)	678.07 a	673.11 a
Specific heat ($kJ.kg^{-1}.°C^{-1}$)	1.405 a	1.526 b
Thermal conductivity ($W.m^{-1}.°C^{-1}$)	0.111 a	0.112 a
Thermal diffusivity ($m^2.s^{-1}$)	$1.1689.10^{-4}$	$1.0901.10^{-4}$

[*] Values of means followed by the same letter do not differ statistically from each other (between columns) by Tukey's test at 5% probability ($p < 0.05$).

Source: Authors (2022).

The reduction in the density value between the initial and final samples was approximately 0.73%. This did not represent a decrease in product quality and may have been a function of the variation in the hygroscopic equilibrium of the material.

The mean colorimetric coordinates for each sample, as well as the total color difference (ΔE) between them, are shown in Table 2.

Table 2: Colorimetric coordinates obtained for the samples obtained at the beginning and end of the storage period in a cooled environment and the value of the total color difference between them.

Sample	Colorimetric coordinates			Total color difference(ΔE)
	A	b	L	
Initial	+2.07	+15.66	43.94	1.86
Final	+2.55	+14.13	44.88	

Like the physical properties, the thermal properties were determined for the initial coffee sample and for the coffee stored in a cooled environment. They were also treated only as initial and final samples, respectively.

There was an increase of 0.9% in the thermal conductivity between the samples at the beginning and end of the storage period.

The initial coffee sample and the samples at the end of storage (both in a cooled and natural environment) were subjected to sensory analysis. The mean scores are shown in Table 3.

Table 3: Mean score obtained by the sensory evaluation method of the SCA for the initial and final samples for both storage systems.

Sample	Mean score obtained
Initial	78.0
Final –Cooled storage	77.0
Final - Natural storage	77.0

To present the mean relative error for different regions inside the cocoon (cooled storage), the temperature collection points were divided into 7 regions (Figure 5). Note that the same point can be part of more than one region.

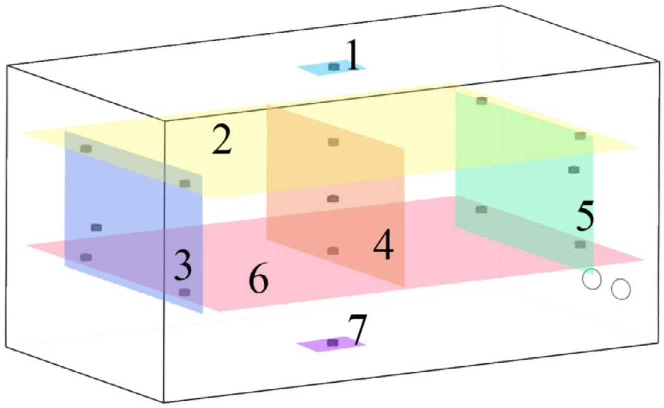

Figure 5: Collection points divided into different regions inside the cocoon for temperature comparison.

Source: Authors (2020).

The mean of the relative errors of the points that covered that region was obtained for each of the 7 regions. The results are shown in Table 4.

For natural storage, Figure 6 shows the overall mean temperature obtained from all sensors throughout the simulation period and the overall mean temperature obtained by the model for the same data collection points.

For the cooled storage, Figure 7 shows the overall mean temperature obtained from all sensors throughout the simulation period and the overall mean temperature obtained by the model for the same data collection points.

Table 4: Mean of the mean relative errors for each region inside the cocoon.

Region inside the cocoon	Mean of the mean relative errors (%)
1	8.23
2	5.46
3	5.07
4	4.41
5	6.48
6	5.48
7	5.73

4 DISCUSSION

There was an increase in water content (in percentage) of approximately 5.85% between the samples, which corresponds to approximately 0.6 (% w.b.). This increase in water content was related to the environmental conditions to which the coffee was subjected during storage.

Analyzing the values obtained regarding the reduction in the bulk density, it was noted a small difference. The reduction in the density value between the initial and final samples was approximately 0.73%. This did not represent a decrease in product quality, according results from sensory evaluation, and may have been a function of the variation in the hygroscopic equilibrium of the material.

In regard to colorimetric analysis, the increase in parameter “a” from +2.07 to +2.55 indicates that there was an increase in red color from the initial to final samples. The reduction in parameter “b” from +15.66 to +14.13 indicates that there was an increase in blue color. Finally, the increase in parameter “L” (lightness) from 43.94 to 44.88 indicates that the sample became slightly lighter, which suggests that bleaching of the stored product occurred.

The total color difference value of 1.86 after 6 months of storage is consistent with the literature, as Afonso Júnior and Corrêa (2003) also obtained a value of approximately 2.0 for the total color difference after 6 months of coffee storage.

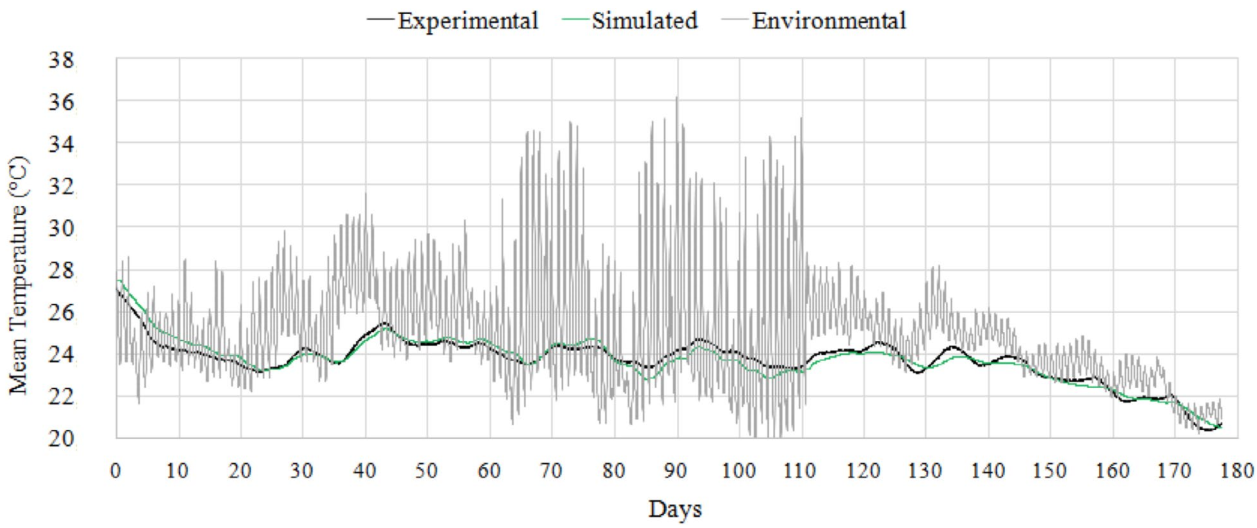

Figure 6: Overall mean temperature obtained experimentally and by the model during storage in a natural environment.

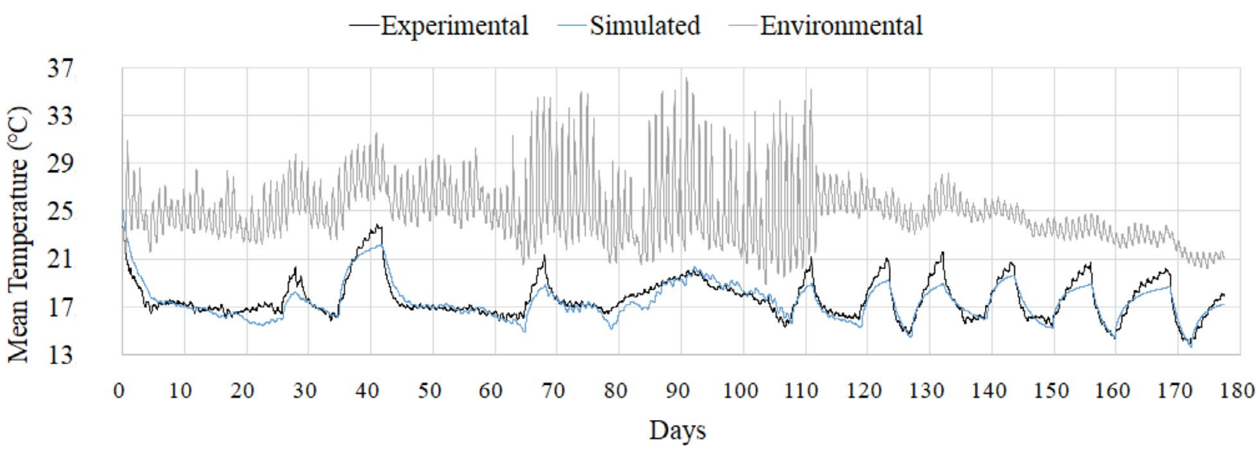

Figure 7: Overall mean temperature obtained experimentally and by the model during storage in a cooled environment.

Bleaching and color change, which occurs as a function of storage conditions, may indicate loss of the initial quality of the grains and cause a product to lose its commercial quality (Coradi; Borém; Oliveira, 2008).

There was an increase of approximately 8.6% in the specific heat value between the beginning and end of the cooled storage. According to Borém et al. (2002), who determined the thermal properties of five coffee varieties and observed that an increase in water content leads to an increase in the grain specific heat, stated that this increase can be explained by the increase in the water content in the product.

A decrease in thermal diffusivity of approximately 6.7% was observed between the samples at the end and beginning of storage. An increase in water content may yield a decrease in thermal diffusivity according to Borém et al. (2002).

There was a quality drop of 1.0 point for both systems at the end of storage, and the quality remained comparable. This may indicate that cooled storage, specifically for the type of coffee used and considering its initial quality, does not lead to a better maintenance of coffee quality than coffee stored only in a natural environment.

According to the temperature modeling, Region 1, which consists of the sensor at the top of the coffee pile, had the highest mean relative error (8.23%), which can be explained by the fact that the sensor was directly in contact with the cooled air that circulated in the interior of the system and because it was the most exposed to external temperature variations; this increased the complexity of the simulation of its temperature distribution. Region 5 had the second highest overall mean relative error (6.48%) because it was the region closest to the cooled air inlets and more susceptible to rapid temperature changes. The other regions oscillated between approximately 4.5 and 5.5%. Despite the aforementioned differences, the simulation result was satisfactory, regardless of the location of the point in the pile.

The mean temperature inside the pile oscillated between approximately 15 and 21 °C throughout most of the storage period and presented an upper limit above the desired value of 18 °C.

5 CONCLUSION

The determination of physical and thermal properties showed that there were significant changes in the water content and specific heat of the samples from the beginning to the end of the storage period in a cooled environment, which are directly related properties. There were no significant changes for bulk density, color, thermal conductivity, or thermal diffusivity. The sensory analysis showed that the quality of the coffee used throughout storage remained the same for both storage systems.

The cooled environment was unable to maintain the temperature within the established limit of 15 to 18 °C, and the temperature in the cooled environment was between approximately 15 and 21 °C. Thus, the system used is not suitable for storage in a cooled environment.

With relative errors lower than 10%, the computational models used were adequate for simulating the functioning of each of the storage systems. It is inferred that numerical simulation can be used to predict the behavior of the temperature distribution of coffee stored in a natural environment and in an environment with cooled air injection. Thus, real conditions can be represented by the computational model, which results in efficiency and savings in experimental processes and thus can be used in other applications.

6 AUTHORS' CONTRIBUTION

RPZ, FSO, and PAR wrote the manuscript and performed the experiment, ETA, FMB, and SDVFR supervised the experiment and co-work the manuscript, and ETA review and approved the final version of the work.

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