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MODELING THE HYGROSCOPIC BEHAVIOR OF COFFEE IN HULL FOR STORAGE OPTIMIZATION

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ABSTRACT

Coffee is one of the most important global commodities, with Brazil leading its production. To ensure its quality and commercial viability, off-season storage is essential. However, inadequate moisture content leads to grain deterioration. The aim of this study was to analyze the hygroscopic behavior of hulled coffee, evaluating mathematical models for predicting moisture adsorption isotherms. The research was conducted using Yellow Bourbon coffee, applying the static method with saturated saline solutions to control relative humidity at temperatures ranging from 10 to 50 °C. Twelve mathematical models were evaluated regarding their fit to the experimental data. The results showed that the adsorption isotherms of hulled coffee follow a sigmoidal pattern, indicating that equilibrium moisture decreases with increasing temperature. The Harkins model presented the best fit, with a coefficient of determination (R^2) of 0.998 and a standard error of estimate (SE) of 0.448, outperforming other widely used models. Visual validation of the model confirmed its high accuracy, with predicted values closely aligned with the experimental data. It is concluded that the Harkins model is the most suitable tool for optimizing the storage of hulled coffee, providing a technical basis for sustainable moisture management and the preservation of grain quality.

Palavras-chave:
Isotermas de sorção
Qualidade do café
Pós-colheita

MODELAGEM DO COMPORTAMENTO HIGROSCÓPICO DO CAFÉ EM COCO PARA OTIMIZAÇÃO DO ARMAZENAMENTO

RESUMO

O café é uma das commodities mais importantes do mundo, e o Brasil se destaca como o principal produtor global. Para garantir a qualidade e a viabilidade comercial do produto, o armazenamento na entressafra é uma etapa fundamental. No entanto, teores inadequados de umidade podem acelerar a deterioração dos grãos. Assim, este estudo teve como objetivo analisar o comportamento higroscópico do café beneficiado, avaliando modelos matemáticos capazes de prever isotermas de adsorção de umidade. A pesquisa foi realizada com café da variedade Yellow Bourbon, utilizando o método estático com soluções salinas saturadas para controle da umidade relativa, em temperaturas entre 10 e 50 °C. Ao todo, doze modelos matemáticos foram avaliados quanto ao ajuste aos dados experimentais. Os resultados mostraram que as isotermas de adsorção do café beneficiado apresentaram comportamento sigmoidal, indicando redução da umidade de equilíbrio com o aumento da temperatura. Entre os modelos testados, o modelo de Harkins apresentou o melhor desempenho, com coeficiente de determinação (R^2) de 0,998 e erro padrão de estimativa (SE) de 0,448, superando outros modelos amplamente utilizados na literatura. A validação visual confirmou a elevada precisão do modelo, com valores estimados muito próximos aos dados experimentais. Conclui-se que o modelo de Harkins é o mais adequado para otimizar o armazenamento do café beneficiado, fornecendo uma base técnica para o manejo sustentável da umidade e para a preservação da qualidade dos grãos.

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INTRODUCTION

Coffee is one of the most traded commodities and one of the most consumed beverages worldwide, with Brazil, Vietnam, and Colombia leading production, and the European Union and the United States as the main importers (ICO, 2024; CONAB, 2025). The market is in constant expansion, driven by consumption in emerging economies and the growing interest in specialty coffees (Abreu *et al*., 2025). In this context of an expanding market, storage emerges as a crucial stage for the sustainability of the production chain, as it ensures the maintenance of grain quality and enables better prices for producers by allowing sales to occur during the off-season (Rosa *et al*., 2022).

Despite its importance, coffee quality is directly influenced by its moisture content which, if inadequate, can lead to chemical, physical, and microbiological deterioration, such as oxidation and microbial growth (Isquierdo *et al*., 2020; Carvalho *et al*., 2024). This hygroscopicity directly affects sensory attributes such as aroma and flavor (Collazos-Escoba *et al*., 2022), and hygroscopic imbalance can compromise the long-term viability of the grain (Rosa *et al*., 2022).

Thus, the concept of hygroscopic equilibrium is central to the conservation of hulled coffee. This state is reached when the water vapor pressure in the grain equals that of the surrounding air, halting moisture exchange between the product and the environment (Carvalho *et al*., 2024; Isquierdo *et al*., 2020). Hygroscopic behavior is precisely described through sorption isotherms, which correlate the grain's moisture content with the equilibrium relative humidity at a given temperature, serving as a basis for creating environments that minimize losses (Zeymer *et al*., 2022; Carvalho *et al*., 2024).

Traditionally, Brazilian producers store coffee in the form of hulled coffee. This practice aims precisely to prolong seed viability and quality, as the dried pericarp acts as a natural protective barrier, minimizing physical and biological damage to the grain (Embrapa, 2004; Simões *et al*., 2022). However, the success of this strategy critically depends on moisture control. Storage conditions without environmental fluctuations, when storage occurs without proper environmental control, may expose the coffee to variations in humidity that compromise this natural protection, leading to quality losses.

This study aims to analyze the hygroscopic behavior of hulled coffee at temperatures ranging from 10 to 50 °C and to identify the most accurate mathematical models for predicting its adsorption isotherms. Fitting these models provides a practical tool to optimize storage, ensuring grain quality and the sustainability of production.

MATERIALS AND METHODS

The study was conducted at the National Training Center for Storage (CENTREINAR), located at the Federal University of Viçosa (UFV), in Viçosa, MG. The coffee samples used, of the Yellow Bourbon variety (Coffea arabica), were harvested at the experimental unit of the Agronomy Department at UFV. After harvest, the coffee was processed using the dry method, keeping the dried husk intact during drying and storage.

Treatments and sampling

To obtain the adsorption isotherms, the static method with saturated saline solutions was employed (Corrêa *et al*., 2014; Zeymer *et al*., 2022). For this purpose, saline solutions such as lithium chloride (LiCl), magnesium chloride ($MgCl_2$), magnesium nitrate ($Mg(NO_3)_2$), and sodium chloride (NaCl) were used, allowing control of water activity (aw) inside the desiccators.

For preparation of the solutions, the salt was added to a volume of distilled water under constant stirring until the solution reached the saturation point. This point was identified when the salt stopped dissolving and formed a precipitate along with a superficial layer of free water, known as the supernatant water film, indicating that the solution had reached its maximum solubility. This film was removed to ensure experimental accuracy.

After solution preparation, three samples of hulled coffee were placed in each desiccator. A hygrometer was used to monitor humidity and ensure that the samples were exposed only to the controlled atmosphere. The assays were conducted at temperatures of 10, 20, 30, 40, and 50 °C.

To describe the hygroscopic behavior of the coffee, the experimental data were fitted to different mathematical models, whose equations are widely applied to agricultural and plant-based products and are presented in Table 1.

Table 1. Mathematical models used for fitting the adsorption isotherms of hulled coffee.

Models	Equations	
Chung- Pfost	Ue = a–b * ln[-(t + c) ln(aw)]	(1)
COP	Ue = exp (a - b* t + c* aw)	(2)
Copace	Ue = exp (a – b * t + c * aw)	(3)
Frend	Ue = a*(aw ^ (1/b))	(4)
Halsey	Ue=exp(a-bt)/-log(aw)^(1/c)	(5)
Harkins	Ue = exp (a-bt)/(c- log(aw))	(6)
Henderson modified	Ue=log(1-aw)/-a*(t+b)^(1/c)	(7)
Oswin modified	Ue=(a+bt)*(aw/1-aw)^(1/c)	(8)
Scop	Ue =exp(a–b + c* exp(aw))	(9)
Sigma Copace	Ue = exp(a–bt)+(c*exp(aw))	(10)
Sigma copace II	Ue = 1/ (at ^ b) + (aw ^ c)	(11)

Where Ue is the hygroscopic equilibrium moisture (%), aw is the water activity on a decimal basis (d.b.), t is the temperature (°C), and a, b, c are the model coefficients.

Source: Corrêa et al., 2014; Zeymer et al., 2022; Zeymer et al., 2023; Silva et al., 2024

Experimental design and statistical analysis

To estimate the parameters and evaluate hygroscopicity, the experimental data were fitted to the mathematical models. The selection of the best-fitting model was based on the highest R^2 value and the lowest values of mean relative error (P) and standard error of estimate (SE) (Azad *et al*., 2023).

Model fitting was performed using nonlinear regression via the Gauss–Newton method (Zeymer *et al*., 2023; Silva *et al*., 2024). All statistical analyses and experimental design procedures were carried out using Statistics version 6.

RESULTS AND DISCUSSION

The validation of the mathematical models, essential for predicting the isotherms, showed high correlation with the experimental data. The Harkins model stood out as the most suitable for describing the hygroscopic behavior of hulled coffee, presenting the lowest estimated mean error and the highest coefficient of determination among all evaluated models (Tables 2 and 3).

The statistical analysis demonstrated that the Harkins model was the most accurate for describing the hygroscopic behavior of hulled coffee. The following equation presents the fitted coefficients for the Harkins model:

$$Ue = \exp(3.065 - 0.007t) / -\log(aw)\hat{}(1/0.517) \quad (13)$$

Figure 1 shows the values estimated by the Harkins model, demonstrating a sigmoidal pattern typical of agricultural products and revealing that, for the same water activity, the moisture content of coffee decreases as temperature increases.

The moisture adsorption isotherm of hulled coffee, with its sigmoidal shape, is consistent with the results of other studies on the hygroscopic behavior of coffee. Dos Santos *et al*. (2020) observed the same pattern in processed coffee beans, and Ordoñez *et al*. (2018) in parchment coffee. This characteristic was also found in seeds of Coffea canephora Pierre (Bustos-Vanegas *et al*., 2018), suggesting that the shape of the isotherm curve is an intrinsic property of the grain, regardless of processing type or the presence of the pericarp.

This behavior is vital for storage because at higher temperatures, the kinetic energy of water molecules increases, facilitating their exit from the grain (Zeymer *et al*., 2023). Thus, even in environments with seemingly high relative humidity, coffee may lose water, compromising its mass and quality.

The accuracy of the Harkins model was confirmed by the residual analysis, which showed excellent agreement between experimental and estimated values. This validation makes the model a highly relevant tool, as it allows producers to predict the ideal moisture content of coffee under different temperature and humidity conditions. This capacity for managing the storage environment is crucial for preventing mass loss and microbial growth, ensuring long-term product quality.

Table 2. Coefficients of the mathematical models used for fitting the adsorption isotherms of hulled coffee

Models	Model variables		
	a	b	c
Chung P-foste	44.123	7.622	40.619
COP	1.982	0.008	1.739
Copace	1.982	0.008	1.739
Frend	28.000	1.161	-
Halsey	5.296	0.014	2.020
Harkins	3.065	0.008	0.517
Henderson modified	0.000	46.163	1.842
Oswin modified	17.036	-0.100	2.715
Scop	1.173	0.007	0.991
Sigma-copace	1.173	0.007	0.991
Sigma-copace II	0.070	-0.009	119.740
Smith	9.219	0.110	11.200

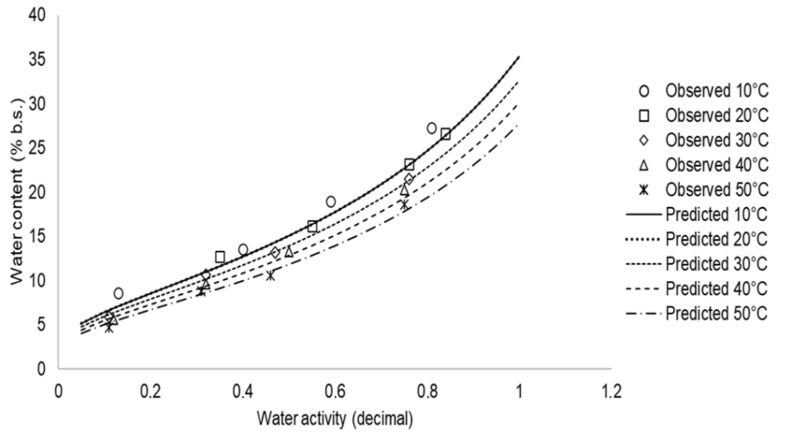
Source: the authors

Table 3. Statistical parameters and residual distribution trends of the mathematical models evaluated for the adsorption isotherms of hulled coffee

Models	Statistical parameters			
	R^2	P	SE	Trend
Chung P-foste	0.99	10.41	0.623	No
COP	0.99	10.75	0.595	No
Copace	0.99	10.75	0.595	No
Frend	0.95	35.37	2.041	Yes
Halsey	0.99	15.01	0.951	No
Harkins	0.99	7.88	0.448	No
Henderson modified	0.97	9.31	0.605	No
Oswin modified	0.99	8.94	0.537	No
Scop	0.99	16.08	0.955	No
Sigma- copace	0.99	16.08	0.955	No
Sigma- copace II	0.97	78.79	6.120	Yes
Smith	0.99	11.19	0.653	No

Where P is the mean relative error, SE is the standard error of estimate, and R^2 is the degree of residual dispersion.
Source: the authors

Figure 1. Moisture adsorption isotherms of hulled coffee at different temperatures.



Source: the authors

CONCLUSIONS

- This study concluded that the Harkins model is the most suitable for describing the hygroscopic behavior of hulled coffee. The analysis revealed that the adsorption isotherms exhibit a sigmoidal pattern and that the grain's equilibrium moisture content decreases with increasing temperature. The predictive ability of the Harkins model provides a crucial technical tool for optimizing moisture management and preserving coffee quality during storage.

AUTHORSHIP CONTRIBUTION STATEMENT

SILVA, W. O. A.: Formal Analysis, Methodology, Validation, Writing – original draft, Writing – review & editing; **CORRÊA, P. C.:** Writing – original draft, Writing – review & editing; **LEITE, R. A.:** Writing – original draft, Writing – review & editing; **CAMPOS, R. C.:** Funding acquisition, Project administration, Supervision, Writing – original draft, Writing – review & editing.

DECLARATION OF INTEREST

The authors declare that they have no financial or personal interests that could influence

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