

Water adsorption isotherms of coffee *blends***Isotermas de adsorção de água em *blends* de café**

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ABSTRACT

This work aimed to evaluate the adsorption isotherms of roasted and grinded coffee, in different blends and storage temperatures. Crude grain coffee of two species were used: arabica (*Coffea arabica*) and robusta (*Coffeacanephora*), dehulled and dried. Grain were submitted to a selection to eliminate deteriorated grain, damaged and bored, to obtain a homogeneous raw material, without defects. Grain coffee from both species, after triage, were sent to roasting process at medium light level (Agron SCAA#65). After roasting process, grain was processed in a Mahlkönig mill, at average particle size (0.84 m). Blends were made in the following proportions of arabica and robusta: 80:20; 60:40 and 40:60. Samples were stored in BOD chambers for 6 months and kept at temperatures of 10 and 30 °C, with initial moisture content of 2.0 ± 0.3 % (d.b.). At the beginning of storage (time zero) and at 30, 60, 120 and 180 days of storage, moisture content and water activity were determined. Several mathematical models, frequently used to represent the agricultural products hygroscopicity, were fitted to experimental data of sorption. Values of water activity and moisture content varied between 0.1912 and 0.5160; 2.20 and 5.51 % (d.b.), respectively. Modified Oswin model was the one that best represented the adsorption of coffee blends.

Keywords: mathematical modeling, moisture content, water activity

RESUMO

Este trabalho teve como objetivo avaliar as isotermas de adsorção de café torrado e moído, em diferentes formulações de *blends* e temperaturas de armazenamento. Foram utilizados grãos de café cru de duas espécies: arábica (*Coffea arabica*) e robusta (*Coffeacanephora*), descascados e secos. Os grãos foram submetidos a uma triagem para eliminar os grãos deteriorados, danificados e brocados, a fim de se obter uma matéria-prima homogênea e isenta de defeitos. Os grãos de café de ambas as espécies, após a triagem, foram encaminhados para o processo de torrefação ao nível média clara (Agron SCAA#65). Após o processo de torrefação, os grãos foram processados em moinho Mahlkönig, na granulometria média (0,84 mm). A formulação dos *blends* se deu nas seguintes proporções de arábica e robusta: 80:20; 60:40 e 40:60. As amostras foram armazenadas em câmaras BOD durante 6 meses e mantidos às temperaturas de 10 e 30 °C, com teor de água inicial de cerca de $2,0 \pm 0,3$ % (b.s.). No início do armazenamento (tempo zero) e aos 30, 60, 120 e 180 dias de armazenamento foram determinadas o teor de água e a atividade de água. Aos dados experimentais de sorção foram ajustados diversos modelos matemáticos frequentemente utilizados para representação da higroscopicidade de produtos agrícolas. Os valores de atividade de água e teor de água variaram entre 0,1912 e 0,5160; 2,20 e 5,51 % (b.s.), respectivamente. O modelo de Oswin modificado foi o que melhor representou a adsorção de *blends* de café.

Palavras-chave: atividade de água, teor de água, modelagem matemática

1 INTRODUCTION

Brazil is the main producer and exporter of crude grain coffee and the second consumer of coffee in the world, being 6.02 kg of green coffee or 4.82 kg of roasted coffee, per person per year (ABIC, 2018). Two species of greater importance for world commerce of coffee are used: *Coffea arabica* L. and *Coffeacanephora*, known as arabica and robusta coffee, respectively.

In Brazil, arabica coffee is the most produced specie, however, robusta coffee is increasing its share, being used as blends along with arabica coffee (Botelho et al., 2016). Blends among arabica and robusta coffees may be accomplished with the objective to exploit sensorial potential of

both species, combining them to enrich flavor and aroma of the final product, according to the target market. Previous work reported the chemical composition and physical properties of arabica and robusta coffee (Botelho et al., 2016; Corrêa et al., 2016a; Corrêa et al., 2016b; Oliveira et al., 2014; Oliveira et al., 2015), however, it was not found at the specialized literature information regarding the impact of blends over storage.

Storage should be performed properly, in which temperature and relative humidity of the environment surrounding the product are important parameters to be considered during storage. They determine the water activity (a_w) of the product and, thus, the water exchange between the product, which is hygroscopic, and the environment (Oliveira et al., 2017). This interaction may be studied through the sorption isotherms.

Sorption isotherms are indispensable to determine and analyze water sorption changes during storage and can be expressed by mathematical models, which differ in their theoretical or empirical basis and the numbers of parameters involved. These models are essential to the prediction and simulation of the performance of materials subjected to a specific process.

The prediction of moisture gain or loss during storage impacts directly at post-harvest procedures for safe storage of the product, affecting its final cost (Corrêa et al., 2016a). Moreover, this information helps to plan actions to prevent and mitigate possible insect and microorganism infestation, as well as assuring higher profitability through control of prices (Oliveira et al., 2014). Storage of roasted and grinded coffee is not indicated due to grinding promotes a higher interaction between the product and the environment, leading to a higher loss of the constituents, thus, the product quality. However, storage of roasted and grinded coffee may occur due to market difficulties, the need of storage due to lack of transportation, prices that are not suitable its immediate commercialization and the need of blends composition at the industry. Thus, hygroscopic equilibrium data will aid the decision making regarding post-harvest procedures of coffee, roasted and grinded, specially at storage and commercialization stages (Goneli et al., 2013).

Given the above-described considerations and the importance of knowledge of the hygroscopicity of agricultural products, this work had the objective to evaluate the hygroscopic equilibrium of coffee blends, through sorption isotherms, in different storage temperatures, throughout storage for 180 days.

2 MATERIAL AND METHODS

Peeled and dried raw coffee beans of *Coffea arabica* L. and robusta (*Coffea canephora*) were purchased at the local market in Manhuaçu, MG. Coffee beans were sorted to remove

deteriorated, damaged, and bored coffee beans to obtain a homogeneous raw material with minimum defects. Afterwards, coffee beans were subjected to the roasting process.

A 300-g raw-coffee capacity preheated, liquefied petroleum gas direct roaster with a rotary cylinder operated at 45 rpm was used to roast the coffee. The degree of roasting was determined by a trained professional by monitoring the sample color and comparing it with the Roast Color Classification System. One roasting degree was used: medium light (Agtron number SCAA#65). Following the roasting process, the coffee beans were processed in a Mahlkönig mill at medium particle size (0.84 mm).

Blends were then formed at the following proportions of arabica and robusta coffee, respectively: 80:20; 60:40 and 40:60. Samples were then placed in polypropylene bags and refrigerated at biochemical oxygen demand chambers in two storage temperatures (10 and 30 °C). Samples were analyzed at five time points (0, 30, 60, 120, and 180 days) over the course of six months, being measured moisture content and water activity.

Moisture content was determined gravimetrically using a forced-air oven at 105 ± 1 °C for 24 h, in triplicate (Brasil, 2009). Moisture content of a coffee sample obtained in each storage period (0, 30, 60, 120, and 180 days) was defined as the equilibrium moisture content, because the samples were stored in permeable plastic bags and the time elapsed was deemed sufficient to reach equilibrium. Water activity (a_w) of the roasted ground coffee samples were assessed using an AquaLab 4TE water activity meter with an a_w accuracy of ± 0.003 . Five replicates were measured.

Mathematical models commonly used to describe sorption phenomena in agricultural products were fitted to the collected hygroscopic equilibrium data (Table 1).

Table 1. Mathematical models used to represent sorption isotherms

Model name	Model	Reference
Copace	$U_e = \exp[a - (bT) + (ca_w)]$	CORRÊA et al. (1995) (1)
Halsey	$U_e = \left[\frac{\exp(a - bT)}{-\ln a_w} \right]^{1/c}$	HALSEY (1948) (2)
Modified Oswin	$U_e = (a + bT) \left(\frac{a_w}{1 - a_w} \right)^{1/c}$	OSWIN (1946) (3)
Sigma-Copace	$U_e = \exp\{a - (bT) + [c \exp(a_w)]\}$	CORRÊA et al. (1995) (4)

in which: U_e = equilibrium moisture content, % d.b.; a_w = water activity, dimensionless; a, b, c = model parameters, which depends on the product; and, T = temperature, °C.

To fit the mathematical models, a non-linear regression was made, using the Gauss Newton method, with the aid of the *software* STATISTICA 8.0[®]. To assess the suitability of the models, the standard deviation of the estimate (SDE), meanrelative error (MRE) and adjusted determination coefficient (R²) (explained variance) values were analyzed. The adequacy of the models was also evaluated by the analyses of the residuals. The SDE and MRE values of each model were calculated using Equations 5 and 6.

$$SDE = \sqrt{\frac{\sum_{i=1}^n (Y - \hat{Y})^2}{GLR}} \quad (5)$$

$$MRE = \frac{100}{n} \sum_{i=1}^n \left(\frac{|Y - \hat{Y}|}{Y} \right) \quad (6)$$

in which: MRE = mean relative error, %; SDE = standard deviation of the estimate, % d.b. Y = observed value, % d.b.; \hat{Y} = estimated value by the model, % d.b.; n = number of observed data; and, GLR = residue degrees of freedom (number of observed data minus number of model parameters).

3 RESULTS AND DISCUSSION

Table 2 present the coefficients of the models fitted to the observed data for the hygroscopic equilibrium of coffee beans blends. The corresponding R², SDE, and MRE values are listed.

Table 2. Parameter estimates of hygroscopic equilibrium models of coffee blends and its respective determination coefficients (R²), SDE and MRE

Models	Blend (arabica:robusta)	Fitted parameters			MRE (%)	SDE (% d.b.)	R ² (%)	Residual Plot
		a	b	c				
Copace	80:20	-0.4058 ^{ns}	-0.0067 ^{ns}	4.1277 [*]	7.91	0.45	88.54	Random
	60:40	0.1808 ^{ns}	-0.0053 ^{ns}	2.7285 [*]	7.80	0.45	86.47	Random
	40:60	0.3445 ^{ns}	-0.0083 ^{ns}	2.3310 [*]	10.60	0.58	81.43	Random
Halsey	80:20	0.7404 [*]	-0.0044 ^{ns}	0.6646 [*]	7.92	0.45	88.50	Random
	60:40	1.2150 [*]	-0.0054 ^{ns}	1.0232 [*]	7.84	0.45	86.40	Random
	40:60	1.4549 [*]	-0.0102 ^{ns}	1.2081 [*]	10.61	0.58	81.40	Random
Modified Oswin	80:20	5.0812 [*]	0.0406 ^{ns}	1.0610 [*]	7.91	0.45	88.74	Random
	60:40	4.5631 [*]	0.0288 ^{ns}	1.6524 [*]	7.21	0.43	87.93	Random
	40:60	4.4351 [*]	0.0439 ^{ns}	1.9415 [*]	9.61	0.53	84.02	Random
Sigma-Copace	80:20	-3.0307 [*]	-0.0065 ^{ns}	2.8630 [*]	7.93	0.46	88.29	Random
	60:40	-1.5437 [*]	-0.0050 ^{ns}	1.8847 [*]	8.59	0.48	84.85	Random
	40:60	-1.1114 ^{ns}	-0.0085 ^{ns}	1.5917 [*]	11.51	0.62	78.77	Random

ns: non-significant by the t-test at 5% of probability

*: significant by the t-test at 5% of probability

At Table 2, it is observed that mathematical models used to describe hygroscopicity presented elevated values of determination coefficient (R^2), higher than 78%. However, R^2 is not enough to prove the fitting quality of a non-linear model, being used mainly for indicative purposes. Thus, the analysis of MRE, SDE, and residual plots are required for non-linear models. Regarding the suitability of a specific model for describing a phenomenon, MRE values lower than 10% indicate a good fit for practical purposes (Samapundo et al., 2007). The ability of a model to reliably describe a specific physical process is inversely proportional to the SDE value (Draper and Smith, 1998). An analysis of the residuals is commonly performed to ensure that a selected model can describe the evaluated phenomenon, in which random distribution indicates a suitable model to represent the phenomenon (Corrêa et al., 2014).

According to the statistical parameters results, the model that best represents the hygroscopic equilibrium of coffee blends is the Modified Oswin. This model presented MRE values below 10%, lower values of SDE, higher values of R^2 and random distribution of the residuals. Baptestini et al. (2017) also indicated that this model was suitable to predict sorption isotherms of roasted and ground coffee. Figure 1 presents the mean values of equilibrium moisture content of coffee blends and its respective sorption isotherms throughout the Modified Oswin model, at temperatures of 10 and 30 °C.

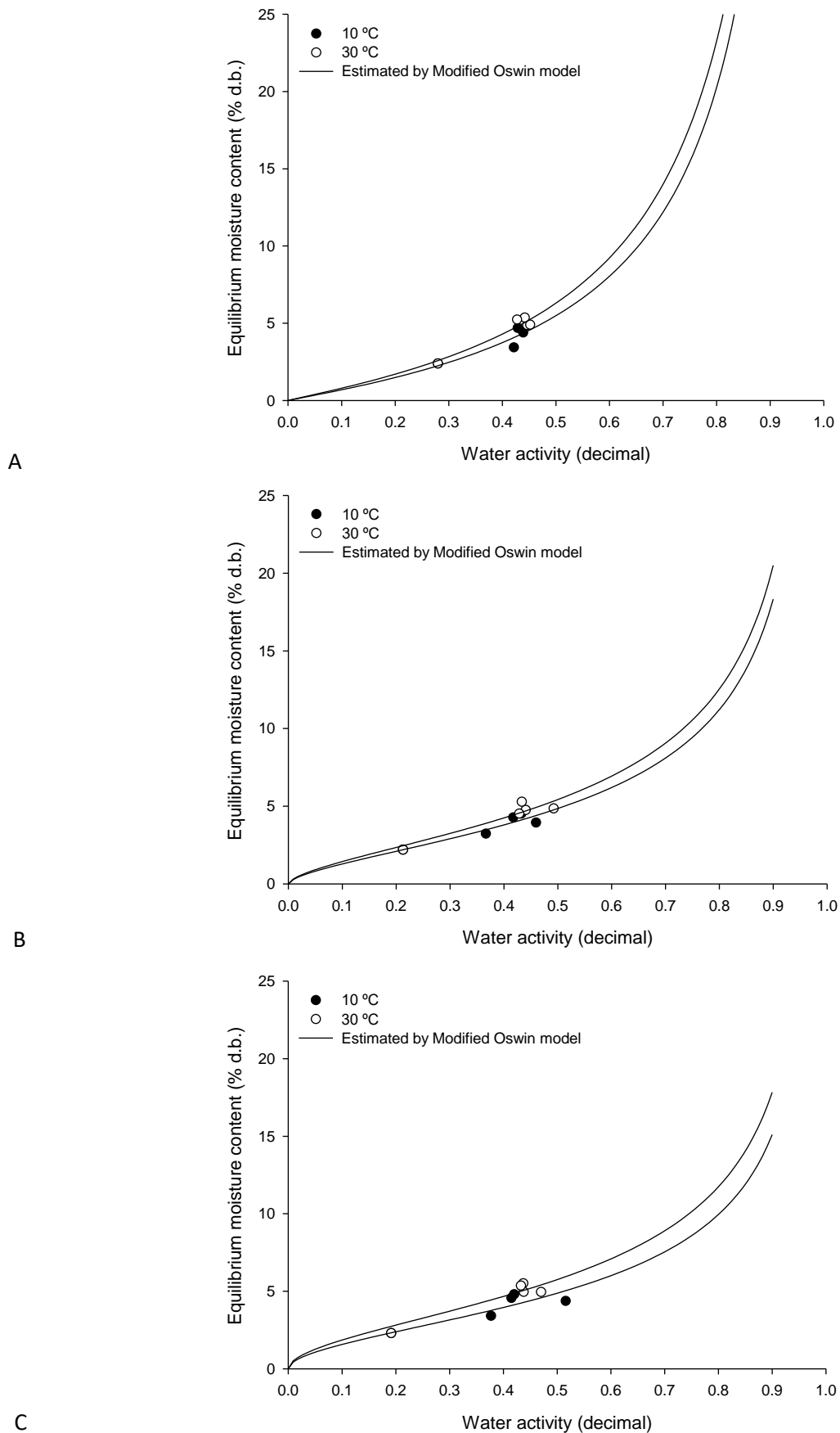


Figure 1. Observed and estimated values, through Modified Oswin model, of equilibrium moisture content of coffee blends (A – 80:20; B – 60:40; C – 40:60), stored at 10 °C and 30 °C

The analysis of the isotherms presented in Figure 1 indicates that the storage temperature affects the hygroscopicity of coffee blends, regardless of the percentage of each coffee species. To reach a given equilibrium moisture content, the water activity should be increased as the temperature increases. Similarly, at a given constant water activity, the equilibrium moisture content decreases with a decrease in storage temperature.

According to Mohsenin (1986), as the temperature increases, molecular vibrations also increase, thereby increasing the distance between molecules and, consequently, decreasing the attractions between molecules, leading to changes of amount of water adsorbed due to temperature alterations at a given relative humidity. Palipane and Driscoll (1992) have demonstrated that an increase in temperature increases the energy levels of water molecules, rendering them less thermodynamically stable and, consequently, facilitating the breaking of the bonds between water and sorption sites, which results in a decrease in the moisture content of the product.

A good correspondence was observed between the data estimated using the Modified Oswin model and the observed data (Figure 1). It was not observed a significant difference, during storage, among adsorption isotherms of coffee blends, indicating that the final chemical composition did not alter the hygroscopic equilibrium of coffee blends (Figure 1).

According to the shape-type of the adsorption isotherm presented in Figure 1, these isotherms may be classified as type III isotherms, according to the classification reported by Brunauer (1945). Type III isotherms present a sharp increase of moisture content in its final portion (Figure 1), corresponding to higher values of water activity. This trend was also reported by Oliveira et al. (2017), due to the high capacity of coffee blends to adsorb water from the environment. There is an increase of water activity throughout storage, from 0.192 at the beginning of storage to 0.5196 after 180 days of storage, regardless of coffee blends.

4 CONCLUSIONS

Storage temperature influences directly the hygroscopicity of coffee blends, independently of arabica and robusta proportions. Blends composition did not alter the adsorption isotherms, which presented an increment of moisture content and water activity throughout storage. The Modified Oswin model is the model that represents best the hygroscopicity of coffee blends.

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