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Mathematical Modeling of Convective Drying Acerola (*Malpighia emarginata*) Residue in Different Thicknesses

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The increasing demand and processing capacity of the fruit processing industries generates a huge amount of waste. Brazil stands out as a producer and exporter of acerola (*Malpighia emarginata*). One of the alternatives to add value to this by-product and contribute to minimizing environmental impacts from its disposal is drying. The drying was carried out with forced air circulation at a speed of 2,20 m s⁻¹ and a temperature of 75 °C, in thicknesses of 3, 4, 5 and 6 mm. The adjustment of the models to the experimental data was performed with Software Statistica 10.0. The effective diffusion coefficient, in the order of 10^{-10} m² s⁻¹, is adequate and did not present a significant difference, among the three major thicknesses. Drying parameters of design and operation were analyzed by mathematical models of Page, Lewis and Midilli, using performance indicators as accuracy (A_f) and noise factors (B_f), mean square error (RMSE) and standard error of prediction (% SEP), associated with each model. All the models present a good adjustment. Despite the greater accuracy of the Midilli model, the Page model is considered more appropriate for process purposes, since it is necessary to adjust only two parameters.

1. Introduction

Brazil stands out as one of the largest producers in the agribusiness sector, with acerola being one of the fruits of growing importance and progressive expansion of the cultivation area, leading the country to the top of the world production ranking (Malegori et al., 2017).

Acerola (Malpighia emarginata), also known as Antillean cherry, West-Indian cherry or Barbados cherry, is a fruit native to Central America, Northern South America and the Antilles (Rezende et al., 2017). The economic interest in its culture is mainly due to its high amount of vitamin (695 a 4827 mg 0.01 g⁻¹), also presenting high levels of other antioxidants, such as carotenoids, bioflavonoids, anthocyanins and phenolics compounds (Mezadri et al., 2008; Rezende et al., 2018). The fruits of the acerola are industrially processed into juices and pulps, food supplements and pharmaceutical products (Almeida et al., 2014), serving multiple markets, which adds even more value to acerola's fruit growing, increasing its demand. In this context, with the increase of production due to the improvement of industrial processing techniques, an enormous amount of organic waste is generated in concomitantly, approximately 40% of the volume of fruit used (Duzionni et al., 2013), composed basically of bagasse, kernels and seeds, which are generally rejected because they are considered of no commercial value and can generate a series of environmental problems when they are improperly discarded (Nóbrega et al., 2015). The acerola residue still presents high concentrations of bioactive compounds, as well as fruit pulp (Rezende et al., 2017) and their non-reuse represents a loss of raw material and energy, since they present enormous potential for applications such as food supplements (Sancho et al., 2015). They may also contain more than 80% of water (Silva et al., 2016), which allows the occurrence of undesirable biochemical reactions that cause the degradation of the material, limiting their shelf life, besides allowing microbiological contamination. Aiming at a better possible alternative for the reuse of these wastes, it is necessary to subject them to a dehydration process (Sanmartin et al., 2017).

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According to Ranganathan et al. (2015), the drying kinetics study allows, through empirical equations and measures such as drying rate, moisture content, temperature and drying time, to predict the drying parameters and behavior of the materials under other conditions, describing the phenomenon of unified form, independently of the control mechanisms. The use of mathematical modeling in the process kinetics allows to estimate parameters that significantly influence the operational energy cost, such as the batch drying time. These models are based on laws of heat transfer and mass, such as Newton's cooling law, considering the external resistance to the transport of moisture between the material and atmospheric air, thus providing a greater extension of accurate results. The semi-theoretical models of Lewis, Page and Midilli are some of the most widely used (Onwude et al., 2016).

The validation of the models used is performed through the use of statistical indicators, which evaluate the ability of each to fit the experimental data, attesting its effectiveness in providing an adequate prediction of the behavior of the drying process (Soares, 2014).

As a way to understand this process and to determine the important parameters of design and operation of the dryer, this study aimed to analyze the mathematical models of Page, Lewis and Midilli to indicate what best suits conditions of convective drying in different layer residues thicknesses, with the aid of performance indicators: mean square error (RMSE), standard error of prediction (% SEP), factor of bias (B_f) and factor of precision (A_f), associated with each model.

2. Methodology

The study was developed at the Laboratory of Innovation in Drying (LIS) of the Food Technology Department at Federal University of Sergipe, in São Cristóvão, Sergipe, Brazil. The residues of green acerola used in the experiments came from Duas Rodas Industry, a fruit processing company located in in the municipality of Estância, Sergipe.

The residue was obtained after the industrial processing, frozen immediately in 10 kg containers, and transported to the laboratory, where it was separated into small batches.

To carry out the research, the samples were distributed in pre-weighed plates, their thickness adjusted with a pachymeter and their masses weighed in analytical balance. The plates were then placed in a dryer (model TE - 394/2) with forced air circulation at a speed of 2.20 m s⁻¹ in a temperature of 75 °C, and weighed at predefined time intervals up to constant weight. The experiments were performed in duplicate and the thicknesses used were 3, 4, 5 and 6 mm.

The data obtained were used to construct the experimental drying curve. For the mathematical modeling, the moisture ratio was determined according to Eq(1), using the experimental data on dry basis.

$$RM = \frac{X_{(t)} - X_{eq}}{X_0 - X_{eq}}$$
(1)

where $X_{(t)}$ consists in moisture at time t, X_{eq} in moisture balance, and X_0 the initial moisture content.

The experimental data of the ratio of moisture were used to fit the Lewis, Page and Midilli models, represented by Eq(2), Eq(3) and Eq(4), respectively. STATISTICA ® version 10.0 software was used to perform the parameter estimation of the models of Lewis, Page and Midilli respectively:

$$RM = exp(-kt) \tag{2}$$

$$RM = exp(-kt^n) \tag{3}$$

$$RM = a \exp(-kt^n) + bt \tag{4}$$

Where *k* is a drying constant (min⁻¹), *t* is the time (min), *n* is an internal resistance, and *a* and *b* the constants of the Midilli model.

The parameters of the models were obtained through non-linear regression and the selection of the most appropriated model was done by performance indicators, using the software Excel® version 2007 for Windows. According to Ross (1996), the Root Mean Square Error (RMSE), shown in Eq(5), is a measure of how spread out these residuals are, i.e., compares the observed and predicted values. The model that best represents the experimental data should present a reduced value for this indicator.

$$RMSE = \sqrt{\frac{\sum(obs - pred)^2}{n_{samples}}}$$
(5)

The Standard Error of Prediction (%SEP) is defined by the estimated standard deviation of the random error between the observed values and the predicted values, as determined the Eq(6).

$$\% SEP = \frac{100}{mean \ obs} \sqrt{\frac{\sum (obs - pred)^2}{n_{samples}}}$$
(6)

The bias factor (B_f), shown in Eq(7), is the parameter that best evaluates the model performance since it relates to the agreement between the predicted and observed values, being the better model performance when the B_f is closer to 1, as $B_f > 1$ indicates how much a model overpredict the observed data and $B_f < 1$ how underpredict it. The accuracy factor (A_f), represented in Eq (8), indicates the average difference between the predicted and observed data, and thus, the smaller the mean, the more appropriate is the model (Santos et al., 2018).

$$B_f = 10^{\left[\frac{\sum \log\left(\frac{pred}{obs}\right)}{n_{observations}}\right]}$$
(7)

$$A_f = 10^{\left[\frac{\sum \log\left(\frac{pred}{obs}\right)}{n_{observations}}\right]}$$
(8)

The effective diffusivity (D_{ef}), function of temperature and material moisture content, is an important mass transport property in the modeling of the drying process of fruits. It was calculated by the Solver tool in Excel®, using the equation proposed by Fick's second law, with solution for flat plate geometry, according to Eq(9), where *L* is the length (mm).

$$\ln RM = \ln \frac{X_{(t)} - X_{eq}}{X_0 - X_{eq}} = \ln \frac{8}{\pi^2} - \pi^2 D_{ef} \frac{t}{4L^2}$$
(9)

3. Results and Discussion

The Figure 1 presents the experimental data with standard deviations and the data predicted by the different models in the four studied thicknesses. It was observed that there was a good correlation between the values for the four thicknesses, except for the Lewis model, which did not show a good fit. Table 1 shows the estimated values of the model parameters for the applied thicknesses (3, 4, 5 and 6 mm).

Table 1: Parameters of drying patterns of green acerola in different thicknesses

Thickness		3 mm		4 mm				5 m	m	6 mm			
	Lewis	Page	Midilli										
<i>k</i> (min⁻¹)	0.030	0.013	0.015	0.019	0.004	0.005	0.013	0.002	0.003	0.011	0.001	0.001	
n	-	1.223	1.177	-	1.372	1.326	-	1.432	1.315	-	1.426	1.342	
а	-	-	0.996	-	-	0.992	-	-	0.991	-	-	0.989	
b	-	-	-0.00015	-	-	-0.00014	-	-	-0.00029	-	-	-0.00021	

The parameter k values present the same magnitude order for the models studied for each thickness, with exception for Lewis model to high thickness (4 mm, 5 mm and 6 mm). The increase in thickness reduced the value of k, indicating a higher water resistance to diffusion.

The similarity between the Page and Midili models is due to the parameter n. The values of n are reasonably smaller in the Midili model due to the influence of the parameters a and b, making the Midili model more complex to perform the adjustment.

In order to quantitatively evaluate which theoretical model best fits the experimental data, performance indicators were used. The results of the performance indicators are presented in Table 2. The RMSE compares the experimental and predicted values and it is considered as an ideal model that presents a reduced value of this parameter. The lower values obtained were in the Page and Midili models for all thicknesses, while the Lewis model showed greater divergence between the experimental data and predicted for the higher thicknesses (4 mm, 5 mm and 6 mm).



Figure 1: Comparison between the models used for green acerola in thicknesses (a) 3 mm, (b) 4 mm, (c) 5 mm and (d) 6 mm

Thickness		3 mm			4 mm	1		5 mm		6 mm			
	Lewis	Page	Midilli	Lewis	Page	Midilli	Lewis	Page	Midilli	Lewis	Page	Midilli	
RMSE	0.033	0.020	0.018	0.051	0.018	0.015	0.062	0.023	0.016	0.057	0.018	0.015	
% SEP	12.50	7.61	6.74	17.03	6.16	4.93	18.45	6.69	4.64	16.47	6.16	4.93	
B _f	3.46	2.44	0.80	3.15	1.90	0.64	2.65	1.72	0.60	2.51	1.90	0.64	
Af	3.68	2.58	0.92	3.46	2.00	0.73	3.05	1.89	0.64	2.90	2.00	0.73	
$D_{ef} ({ m m}^2{ m s}^{-1})$	3.25.10) ⁻¹⁰		5.00.10 ⁻¹⁰			4.83.1	4.83.10 ⁻¹⁰			5.33.10 ⁻¹⁰		

Table 2: Performance indicators of Lewis, Page and Midilli models in different thicknesses

The standard error of prediction (% SEP) makes analysis of the residual of the models and, because of this, its value must be reduced. It was verified that the Midilli model was better adjusted to the experimental data in the different thicknesses.

The bias factor (B_f) is the parameter that indicates the best performance of the model, and according to Oliveira Junior et al. (2016), the perfect agreement between the predicted and observed values represent a B_f equal to 1. Among the models used, the Midilli model shows the best fit.

The accuracy factor (A_i) establishes the mean difference between the experimental and predicted data, where its increase suggests the low accuracy between estimated and observed values. Therefore, the appropriate model will be the one in which this factor is smaller. In this case, the Midili model presents values considerably smaller than the other models, in the four thicknesses studied. As previously noted, the thickness of 6 mm exhibits a more precise adjustment when compared with the other thicknesses.

From the results, it can be deduced that the Page and Midili models are the ones that best fit the experimental data, regardless of the thickness of the layer of green acerola residue. However, the Page model is more appropriate for process control purposes because it requires only two parameters to adjust the data, offering an adjustment with performance indicators similar to the Midili model.

In the work of Soares et al. (2014), in convective drying of jackfruit at 50 °C for a period of 9 h, the Page model also provided a good adjustment with observed values, as well as other models, for example the Midilli model. However, the Page template was selected because of its simplicity.

The effective diffusivity for the three thicknesses presented values in the order of 10^{-10} m² s⁻¹, with no significant difference between the three thicknesses, close to those obtained by Corrêa et al. (2008) in dehydration process of acerola, 1.80×10^{-10} to 5.98×10^{-10} m² s⁻¹. Gomes et al. (2018) found values of 5.79×10^{-10} and 2.03×10^{-9} m² s⁻¹ for 'jambu' leaves crushed mass effective diffusion coefficients in the thicknesses of 5 and 10 mm, respectively. Nag & Dash (2016) in elephant apple drying showed a diffusion coefficient with a minimum value of $1,095.10^{-10}$ m² s⁻¹, at a temperature of 50 °C, and a maximum value of $2,283.10^{-10}$ m² s⁻¹ at 80 °C. These data are in line with what is stated by Onwude et al. (2016), where over 80% of diffusivity values of fruits and vegetables are in the region 10^{-11} to 10^{-8} m² s⁻¹.

4. Conclusions

It was observed that, among the analyzed models, the Midilli model presented kinetics whose predicted data correlated well with the observed values for the four thicknesses. This choice was made by the performance indicators, but the Page model is considered more appropriate for process purposes, since it is necessary to adjust only two parameters. Regarding the parameters found, *k* was lower for the thickness of 6 mm, probably due to the higher resistance of the layer to mass transfer. The diffusion coefficient presented close values, in the order of 10^{-10} m² s⁻¹.

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