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DETERMINING EFFECTIVE DIFFUSION COEFFICIENT OF BANANAS DURING DRYING PROCESS USING DIFFERENTIAL EVOLUTION

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Abstract. *The objective of this study was to explore, via computational simulation, the capability of an inverse problem method to determine the effective diffusion coefficient of water in banana from experimental data of drying. Heat transfer and moisture at the center of the banana using the explicit 1D FDM with drying temperatures in the range between 17-65ºC and moisture in the range between 0.01-3.43 was investigated. The mathematical model considered the effects of convective heat and mass transfer at surface of fruit. The banana was represented as a homogenous and isotropic fruit material. Assuming one-dimensional drying process and known thermophysical properties of the food material, temperatures were generated at different locations of the banana sample by numerically solving the partial differential equations for heat and mass transfer. The equations systems are solved to obtain solution to the inverse problem. The optimization method, Differential Evolution (DE), was then applied efficiently to find the best coefficients of the effective diffusion coefficient that varies with the moisture. The goal of this optimization method is to reduce the uncertainty and approach essentially unique solution for each case studied*.

Keywords: *Effective diffusion coefficient, FDM, Heat and Mass Transfer, Optimization, Differential Evolution*

1. INTRODUCTION

The drying foods is very important in the present days because as it allows the conservation of foods products by inhibiting microbial growth and enzymatic modification (Carleus *et al.*, 2017) besides facilitating the transport and storage due to the reduction in size (Hayashi, 1989). The drying process is basically peeling the fruit and slicing into slices, and exposing the slices to a stream of hot, dry air. The thickness of the slices, in relation to the length of the diameter, allows to simplify the process of diffusion of heat only, in the radial direction.

The process of mass transfer, and diffusion of heat that occurs concomitantly, and for this work it was analyzed both processes, in a banana. For the formulation of the work it was necessary to consider the geometric simplifications presented in item 2.1 and the physical phenomena that occur during the drying process are: the transport of moisture along with the diffusion of heat from the interior of the fruit towards the stream of dry, warm air surrounding the fruit, and the decrease in the length of the transverse diameter of the fruit; due to loss of water. The mass transport phenomenon is intimately the heat diffusion, due to the evaporation process of the moisture that occurs in the surface of the fruit, so the purpose of this article is to determine the function that describes the behavior of the mass diffusion coefficient, correlated with the temperature evolution obtained experimentally during the whole drying process.

Many physical phenomena are described by differential equations, but their solutions are complex to the analytical resolution. Therefore, another type of evaluation is required, called numerical methods. Numerical methods are a finite sequence of arithmetic operations that approximate the exact solution of the problem. A method such as the finite difference method (FDM), which acts directly on the differential equations, replacing them as derived from the problem by difference formulas. For its good result, FDM is applied in several areas of engineering (Junior *et al.*, 2014), such as structures (Deus *et al.*, 2010).

This paper is organized as follow: section 2 briefly presents the bibliography review about heat and mass transfer and FDM simulation and the case study from the process data, while section 3 describes the method that used for analysis of case study. Section 4 brings the result and discussion between numerical and experimental data. Finally, section 5 concludes about the article and presents future work.

2. THEORETICAL FORMULATION

This section presents the literature reference associated with heat and mass transfer and the simulation to provide an overview of the integration of these themes.

2.1 Heat and moisture transfer

Many of the phenomena that involving energy conservation are complex such as relation between heat and moisture (Mendes, 1997): specific thermal capacity and thermal conductivity being influenced by the moisture and the mass balance being influenced by temperature. Due to complexity, the phenomena involving energy conservation are simplified. The main energy conservation phenomena are adsorption and desorption of moisture, air flow between spaces, conduction of bi and three-dimensional heat and moisture migration in porous elements.

The drying is the operation in which the liquid is removed from the solid material and depends on air temperature, air velocity, material thickness, material pre-treatment, and others (Erenturk & Erenturk, 2007). The drying of a foods, widely used in food industries, is considered as a phenomenon of simultaneous heat and mass transfer (Wojeicchowsli *et al.*, 2015).

For the numerical analysis, a mean approximation of the properties of the external air stream will be considered, which will have the convective coefficient attached to the radius of the fruit, and a moisture gradient of the dry air, in relation to the humid external surface of the fruit. The present study approaches the drying of a banana and takes into account the following approaches:

- The physical properties in the banana are homogeneous;
- The geometry of banana is represented like an infinite cylinder of length L (m) and radius defined between [0; R], with $R \approx 0.015$ (m) as shown in Fig. 1a and Fig. 1b respectively;
- The thermal diffusivity was considered dependent on temperature during drying, that is, varies with temperature;
- The coefficient of mass diffusivity, D_{ef} (m/s^2) is depending on the moisture of the banana, it is the main of this study).

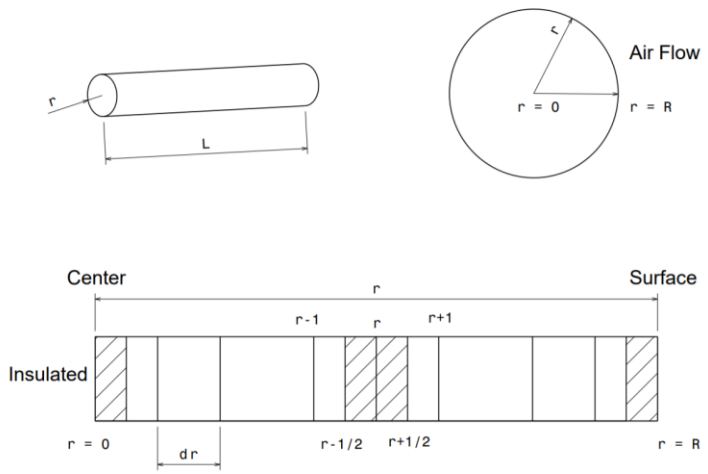

Figure 1. Radial representation of the Banana

The governing equations from the heat and moisture transfer are based on Fouries's law and mass transfer equations described by Fick's unidirectional diffusion equation (Cranck, 1975) and are given by:

$$\frac{\partial T}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(r\alpha\frac{\partial T}{\partial r}\right) \tag{1}$$

$$\frac{\partial X}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(rD_{ef}\frac{\partial X}{\partial r}\right) \tag{2}$$

where, t (s) is the time, r (m) is the transfer direction, α (m/s^2) is the thermal diffusivity, T(K) is the temperature, X is the moisture content, D_{ef} (m/s^2) is the effective diffusion coefficient.

2.2 Boundary Conditions

The initial condition, it was considered that initial temperature and moisture of the banana are uniform, as shown by

$$T(r,0) = T_0 \tag{3}$$

$$X(r,0) = X_0 \tag{4}$$

where, T_0 is the initial temperature in the center of the banana ($r = 0$).

For the boundary conditions to a 1-D problem, it was considered the convective effect heat transfer and moisture at surface, and the condition of symmetry in the center of the fruit.

The Eq. (5) and (6) represent the boundary conditions in relation to the heat diffusion process, at the end and center of the fruit respectively:

$$-k\left.\frac{\partial T}{\partial t}\right)_{r=R} = h(T_R - T_e) + \rho_s \Delta r \frac{\partial \bar{X}}{\partial t}[h_{fg} + c_v(T_R - T_e) \tag{5}$$

$$-k\left.\frac{\partial T}{\partial t}\right)_{r=0} = 0 \tag{6}$$

The Eq. (7) and Eq. (8) represent the boundary conditions in relation to the mass diffusion process, at the end and center of the fruit respectively:

$$-D_{ef}\left.\frac{\partial X}{\partial t}\right)_{r=R} = h_m(X_R - X_e) \tag{7}$$

$$-D_{ef}\left.\frac{\partial X}{\partial t}\right)_{r=0} = 0 \tag{8}$$

where, h (W/m^2 °C) is the heat transfer convective coefficient given by Eq. (9), $\rho_s = 1970$ (kg/m^3) is the dry solid density, $\bar{X} = \frac{1}{R}\int_0^R X(r,t)dr$ is the average moisture content in the section, h_{fg} (J/kg) is the latent heat of vaporization of water obtained by air dry conditions, c_v (J/kg.K) is the specific heat of vapor of water, h_m (m/s) is the mass transfer convective coefficient, X_e is the equilibrium moisture, T_R is the temperature ratio, T_e is the equilibrium temperature (Mariani *et al.*, 2008).

$$h = \frac{kNu}{d} \tag{9}$$

$$Nu = 0.97 + 0.68Re^{0.52}Pr^{1/3} \tag{10}$$

$$Re = \frac{\rho v d}{\mu} \tag{11}$$

where, k (W/m °C) is the thermal conductivity of the banana, Nu is the Nusselt number given by Eq. (10), d is the diameter of the banana, Re is the Reynolds number calculated by Eq. (11), $\mathrm{Pr} = 0.707$ is the Prandtl number, ρ (kg/ m^3) is the air density, v (m/s) is the air velocity of the drying, μ (Pa s) is the air viscosity (Kreith & Bohn, 2003).

The Table 1 shown the air drying conditions and parameters used according Queiroz and Nebra (2001) by 6 experimental cases.

Table 1 – Air drying conditions and parameters used

Cases	T_e (ºC)	h_m (m/s)	X_0	X_e	v (m/s)	h_{fg} (J/kg)	c_v (J/kg.K)	$Time$ (h)
1	29.9	3.19 x 10^{-7}	3.43	0.1428	0.38	2430750	1902.3	121.9
2	39.9	6.96 x 10^{-7}	3.17	0.0554	0.33	2407180	1905.0	72.0
3	49.9	6.94 x 10^{-7}	3.21	0.0579	0.37	2383140	1907.9	40.8
4	60.2	4.96 x 10^{-7}	2.96	0.0426	0.36	2357850	1911.0	35.3
5	60.5	7.50 x 10^{-7}	3.04	0.0211	0.35	2357100	1911.1	27.8
6	68.4	4.99 x 10^{-7}	2.95	0.0121	0.39	2337310	1913.5	27.6

2.3 Finite Difference Method

The purpose of the Finite Difference Method (FDM) is to approximate the differential equations that modeling the problem using discrete points in the domain. The method consists in replacing the derivatives by difference equations. Thus, when more points the problem has (mesh) the better a method accuracy will be. The formulas used for the FDM are obtained by expanding the Taylor series around given point. For the description of the phenomena of heat and mass transport, presenting in this work, will be used the method of the finite differences central as presented (Maliska, 2004).

The partial derivative of the temperature in relation to the time represented by Eq. (2), applied for a given instant of time *j*, and at a position *i*, can be approximated in the discretized form by Eq. (13). The thermal diffusivity term, α (m/s^2), does not vary with the position and with time. The indices $r_{i+1/2}$ and $r_{i-1/2}$ represent an increase and decrease, respectively, in the value corresponding to half of the distances, of the knots of the meshes as observed by Fig 1, added with the location of the radius, denoted by the index r_i. Put it in common words, the distance from the center to the radius, more or less the value of half of the distances between the nodes of the mesh.

The same discretized form approximation can be applied to the partial derivative of temperature with respect to time according to Eq. (2), leading to Eq. (11). Both the diffusion of moisture and heat are free from the additional terms, so the partial derivatives of both quantities (temperature and moisture) with respect to time coincide with the same total derivatives.

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\alpha\frac{\partial T}{\partial r}\right)_{r=0} = \frac{4.\alpha}{\Delta r^2}\left(T_{i+1,j} - T_{i,j}\right) \quad (12)$$

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\alpha\frac{\partial T}{\partial r}\right)_{0<r<R} = \frac{\alpha}{r_i}\left(\frac{r_{i+1/2}T_{i+1,j} - (r_{i+1/2} + r_{i-1/2})T_{i,j} + r_{i-1/2}T_{i-1,j}}{\Delta r^2}\right) \quad (13)$$

$$T(r=R) = \left(\frac{T_{i,j+1} + \frac{h\Delta r}{k}T_e - \frac{\rho_s \Delta r^2}{k}\frac{\partial \bar{X}}{\partial t}(h_{fg} - c_v T_e)}{1 + \frac{h\Delta r}{k} - \frac{\rho_s \Delta r^2 c_v}{k}\frac{\partial \bar{X}}{\partial t}}\right) \quad (14)$$

The Eq. (13) represent the formulation in respect to advance in time using $\Delta t = 0.05$.

$$\left.\frac{\partial T}{\partial t}\right)_{i,j} = \frac{T_{i,j+1} - T_{i,j}}{\Delta t} \quad (15)$$

The moisture distribution field are represented by similar approximation equations, as observed in Eq. (17). As can be seen, differently from the heat diffusivity coefficient α (m/s^2), the coefficient of mass transfer coefficient D_{ef} (m/s^2) depends on the average humidity $\bar{X}$ along the fruit for each time pass, which can be denoted by the subscript index *j*:

$$\frac{1}{r}\frac{\partial}{\partial r}\left(rD_{ef}\frac{\partial X}{\partial r}\right)_{r=0} = \frac{4D_{ef_j}}{\Delta r^2}\left(X_{i+1,j} - X_{i,j}\right) \quad (16)$$

$$\frac{1}{r}\frac{\partial}{\partial r}\left(rD_{ef}\frac{\partial X}{\partial r}\right)_{0<r<R} = \frac{D_{ef}}{r_i}\left(\frac{r_{i+1/2}X_{i+1,j} - (r_{i+1/2} + r_{i-1/2})X_{i,j} + r_{i-1/2}X_{i-1,j}}{\Delta r^2}\right) \quad (17)$$

$$\frac{1}{r}\frac{\partial}{\partial r}\left(rD_{ef}\frac{\partial X}{\partial r}\right)_{r=R} = \frac{4D_{ef_j}}{\Delta r^2}\left(X_{i+1,j} - X_{i,j}\right) + 2h_m\left(\frac{X_{i,j} - X_e}{\Delta r}\right) \quad (18)$$

The process of diffusion of heat, and moisture, occurs simultaneously with the process of reducing the size of the fruit, especially the diameter, due to the loss of water, inherent in the process. The size of the diameter directly influences the distance between the knots, since the number of knots is invariant throughout the drying process and equally thick between them. Another phenomenon observed is the change in the heat diffusion due to the boundary conditions, which are affected by the Nusselt number. The Nusselt number depends indirectly on the diameter of the fruit. According to the (Queiroz & Nebra, 2001), the Eq. (18) calculates the decrease the radius size for each time pass, during the process.

$$R = [0.4721 + 0.1819X_e + 0.1819(\bar{X} - X_e)]R_0 \quad (19)$$

where, R_0 is the initial radius before the process start.

3. INVERSE METHOD

3.1 Differential Evolution - DE

The differential evolution is a bioinspired algorithm based in population denominated optimization metaheuristic. The classic algorithm of DE is the same of genetic algorithm, but it is faster than its predecessor (Pinto, 2016).

The optimization metaheuristics are widely recognized as efficient approaches to solve many optimization problems that do not have exact solution (Boussaïd *et al.* 2013). According DAS *et al.* (2009) in recent years, many approaches of DE have been highlighted in optimization works and in some cases even better results than many other bioinspired algorithm.

Many applications have used the DE algorithm to search for solutions, as in the case of the optimization of the trajectory of a satellite (Ghosh, Chattopadhyay, 2015).

In an extend way, the DE algorithm can be interpreted by the following steps, assuming that the search for the global optimization point is a real parameter in the space R^D:

i. The initial population must be within the lower and upper bounds of each project variable and initialized at random, as shown in Eq. (20)

$$x_{i,g} = x_{i,L} + rand_{g,i}[0,1](x_{i,U} - x_{i,L}) \tag{20}$$

where, i is the individual, g is the generation, $x_{i,L}$ are lower limits of the project variable and e $x_{i,U}$ are lower limits of the project variable and $rand_{g,i}[0,1]$ is the random number generated with uniform distribution in the interval 0 and 1.

ii. Then, the initial population generated must be evaluated by an objective function;

iii. After being evaluated, the population must undergo mutation (DE strategy) using a difference vector and resulting in the perturbation vector. The Eq. (21) show the perturbation vector calculation for the strategy *rand-to-best*/1/*bin*:

$$v_{i,g} = x_{i,g} + F\left(x_{r_1^i,g} - x_{i,g}\right) + F\left(x_{r_2^i,g} - x_{r_3^i,g}\right) \tag{21}$$

where, $x_{r_1^i}$, $x_{r_2^i}$ e $x_{r_3^i}$ are randomly selected vectors of the current population, the indices r_1^i, r_1^i e r_3^i are random integers chosen between $[1, NP]$, F is the weighting factor or weight applied to the difference vector given the Eq. (22) and $v_{i,g}$ is perturbation vector;

$$F = F_m rand(1) + F_m \tag{22}$$

iv. After mutation, the binomial cross of the population must be applied to result in the new diversified generation, as show in Eq. (23):

$$u_{i,g}^{j} = \begin{cases} v_{i,g}\ se\ rand_j\ (0,1) \leq Cr\ ou\ j = j_{rand} \\ x_{i,g}\ caso\ contrário \end{cases} \tag{23}$$

where, *Cr* is the crossing coefficient, and $j = 1,2, \dots D$.

v. And finally, the next step is the selection for the new generation. In the DE the whole population competes with each other, that is, the one with the best value of the objective function is selected for the next generation, as show in Eq.(24):

$$x_{i,g+1} = \begin{cases} u_{i,g}\ \text{se}\ f(u_{i,g}) \leq f(x_{i,g}) \\ x_{i,g}\ caso\ contrário \end{cases} \tag{24}$$

where, $f(x)$ is the objective function will be minimized.

The routine i. until the routine v. must be repeated until it reaches the stop criterion. According by Das (DAS, 2011) the stop criterion can be: 1) iteration numbers (gen_{max}); 2) while the best *fitness* of the population does not change appreciably after successive iteration; and 3) achieve a predefined objective function value.

For optimization of the inverse method was used the MATLAB© code. For a better statistical analysis of the method was run 10 experiments for each case and for the stopping criterion was using equal to 30. The Table 2 shown the DE and FDM parameters used in the simulations.

Table 2 - DE and FDM Parameters

Parameter	Value
D	2
$[x_{i,L}, x_{i,U}]$	$[10^{-13}\ 10^{-11}]$
NP	10
Cr	0.1
F_m	0.1

4. RESULTS AND DISCUSSION

The main of this study is to determine the effective diffusion coefficient using the temperature in the center and average moisture content of the banana. The proposed equation is described as:

$$D_{ef} = a_1 X_m + a_2 {X_m}^2 \tag{25}$$

where, a_1, a_2 are the coefficients, X_m is the average moisture in the instant t for the section given by $X_m = \frac{1}{R}\int_0^R X(r,t)dr$ (kg_w/kg_{dm}), where w is the water and dm is dry matter.

The inverse problem was applied calculating deviations between experimental and simulated temperatures in the center of the banana, and such precision was evaluated calculating the multiple correlation coefficient (Pearson coefficient), given by:

$$R^2 = 1 - \frac{f}{\sum_0^j (T_e - \overline{T}_e)^2} \tag{26}$$

where, T_e is the experimental temperature in the center of the banana, $\overline{T_e}$ is the mean experimental temperature in the center of the banana, f is the objective function used in DE optimization aproach given by:

$$f = \sum_0^j (T_e - T)^2 \tag{27}$$

where, T is the simulated temperature in the center of the banana using difference finite method and j is the final time for each case study.

The best results obtained by the Pearson coefficient and function f are shown in Table 3.

Table 3 - Parameters Eq. (19)

Cases	$a_1 x10^{-11}$	$a_2 x10^{-11}$	R^2	f
1	0.0267	0.0860	0.9958	0.0699
2	0.0100	0.0433	0.9958	0.1463
3	0.2134	0.0100	0.9957	0.0668
4	0.3778	0.0873	0.9960	0.0732
5	0.1805	0.0100	0.9976	0.0760
6	0.0100	0.1015	0.9956	0.3927

The next figures (Fig. 2 to 7) shows numerical and experimental temperatures at the thermal center (r = 0) for the six cases. It’s easy to see that the method applied to predicted temperatures are in excellent agreement with experimental data. These figures show the temperature profiles at the thermal center of infinite cylinder predicted by described method using the parameters of the Table 3, compared with the experimental data for all cases.

So, these results shows the importance of include effective diffusion coefficient depending of the temperature. It’s a numerical study that improve this methodology and turn this analysis better, with more accuracy and with more credibility.

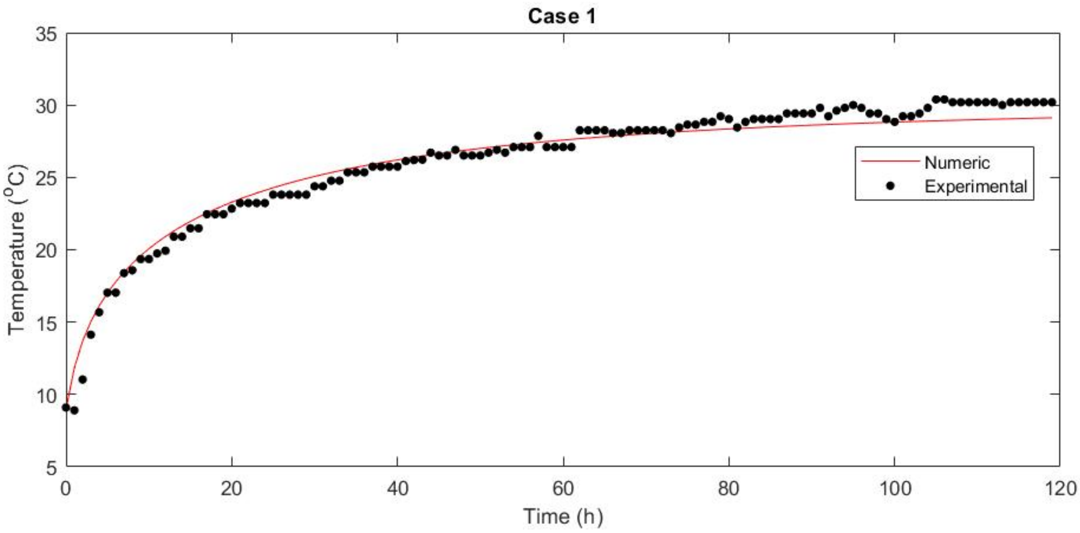

Figure 2 - Experimental validation for the inverse method (central temperature, in r = 0) for the Case 1

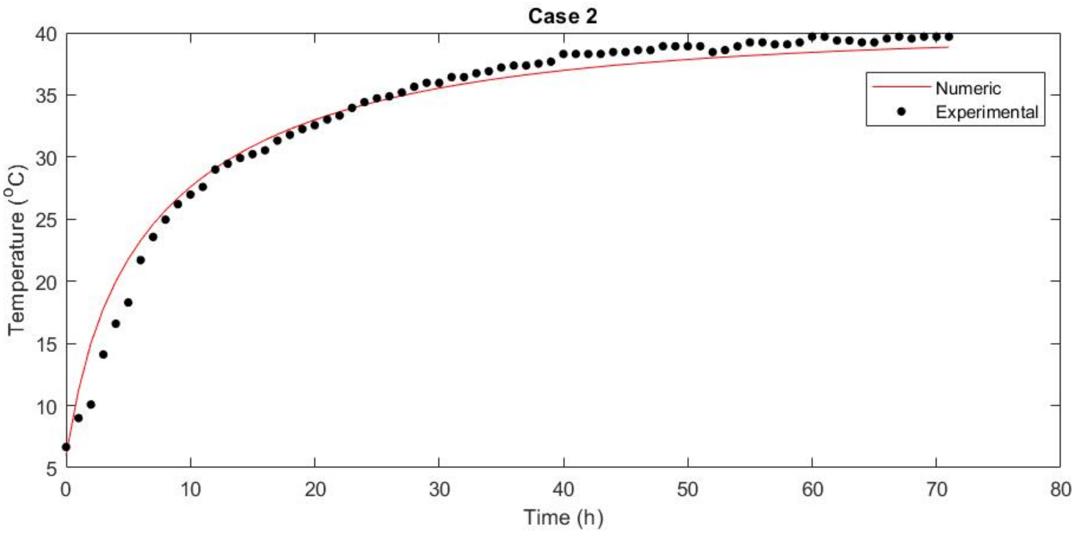

Figure 3 - Experimental validation for the inverse method (central temperature, in r = 0) for the Case 2

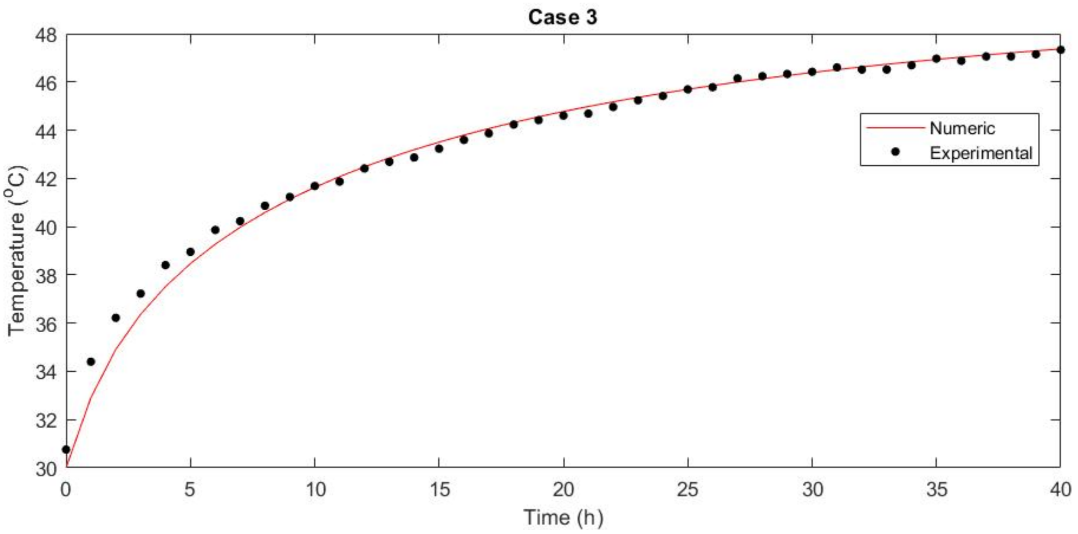

Figure 4 - Experimental validation for the inverse method (central temperature, in r = 0) for the Case 3

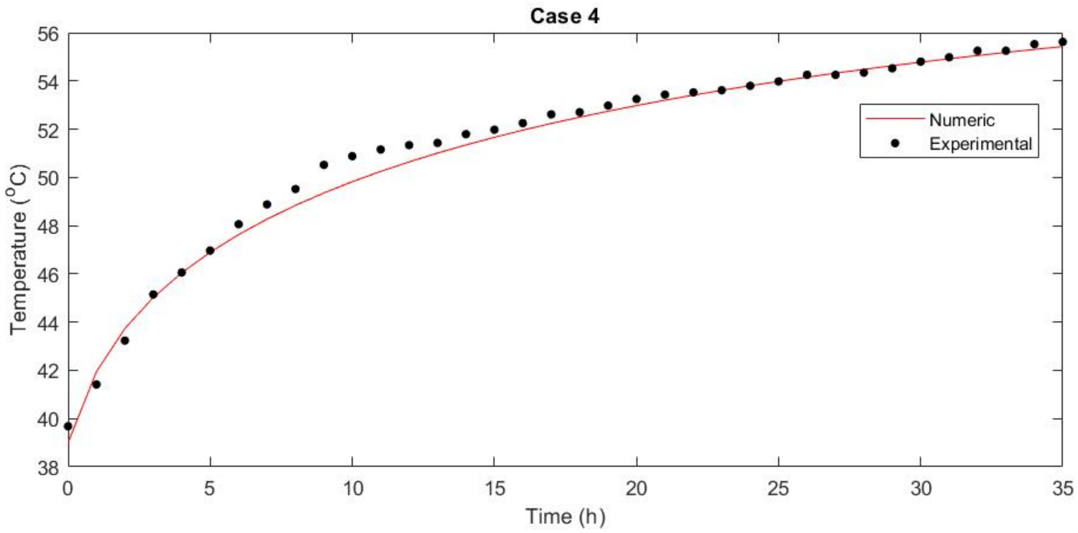

Figure 5 - Experimental validation for the inverse method (central temperature, in r = 0) for the Case 4

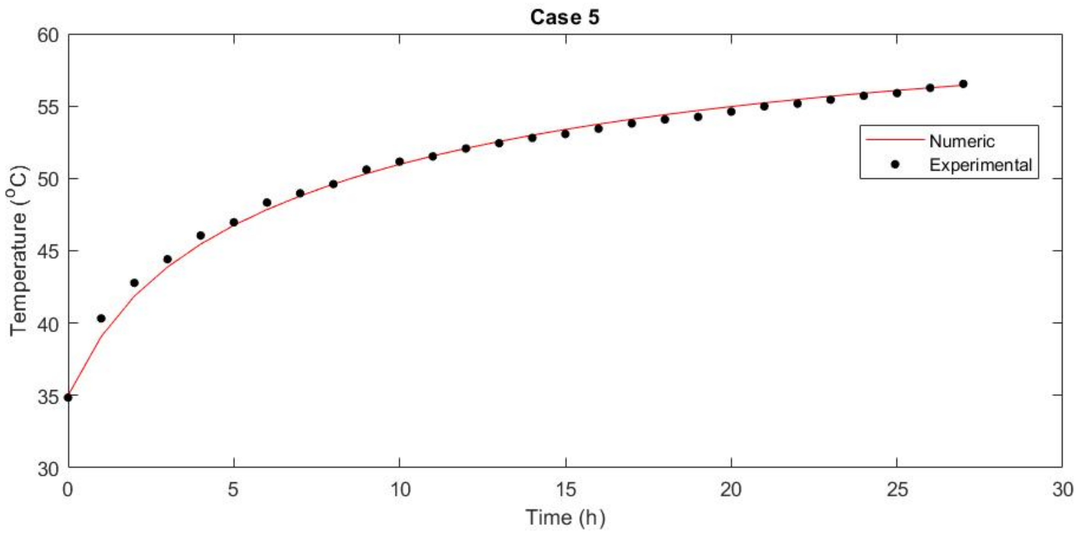

Figure 6 - Experimental validation for the inverse method (central temperature, in r = 0) for the Case 5

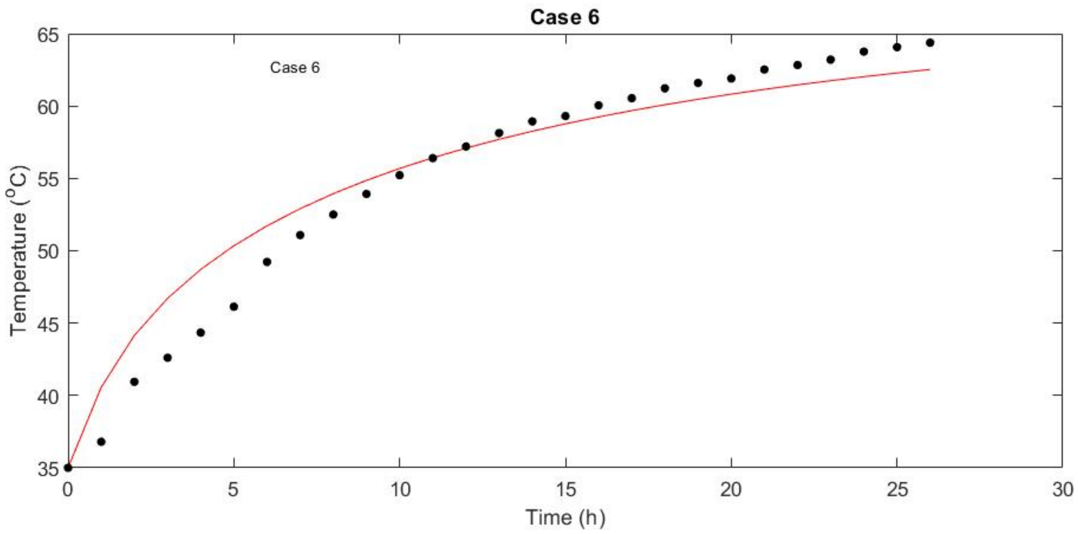

Figure 7 - Experimental validation for the inverse method (central temperature, in r = 0) for the Case 6

There are some differences with other works of the literature due the different values of moisture content (all this results are dependent of moisture content of the food during the process that was submitted), drying temperature, body shape and methodology, so it's acceptable these differences. Then, for the all cases the numerical analysis were verified and approved to predict the thermal profile during drying process.

5. CONCLUSIONS

The inverse method for obtaining the diffusion coefficient function, as a function of the mean humidity along the fruit radius for each step time, was shown to be an extremely efficient method, as observed in the graphs depicted in (Figs. 2 to 7). The mass diffusion coefficient, described as a second-order function, as opposed to a fixed diffusion coefficient throughout the whole process makes the problem more precise than the theoretical data. Although the precision of the binomial expansion of the mass diffusion coefficient function has a direct relation with the higher order, one must take into account the computational processing time for each time step, together with the desired precision, that is, for fruit drying processes, it is not interesting, very precise approximations, since the order of the coefficient even if constant, already presents an extremely low value, besides this fact becomes self-evident, that for very low values, the analysis through the mechanics of the continuum, becomes unfeasible.

For future work, it is proposed an analysis, which relates the mass diffusion coefficient, with the average temperature. It may also be proposed that the fruit can be treated not only as a continuous and compact but rather as a porous medium, another proposal would be to consider the effect of heat exchange through the radiation, which for this work was not properly addressed, a since every approach was applied on top of a linear problem.

6. ACKNOWLEDGEMENTS

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8. RESPONSIBILITY NOTICE

The authors Pinto, Colaço, dos Santos, Batistella and Mariani are the only responsible for the printed material included in this paper.