

DIFFUSION MODELS TO DESCRIBE THE DRYING PROCESS OF PEELED BANANAS: OPTIMIZATION AND SIMULATION

Cleide Maria Diniz Pereira da Silva e Silva cleidedps@uol.com.br

Wilton Pereira da Silva wiltonps@uol.com.br

Josivanda Palmeira Gomes, josi@deag.ufcg.edu.br

Pedro Luiz do Nascimento pln@df.ufcg.edu.br

Universidade Federal de Campina Grande, Rua Aprígio Veloso, 882, Bairro Universitário, Campina Grande/PB Brasil

Vera Solange de Oliveira Farias vera-solange@uol.com.br

Universidade Federal dos Vales do Jequitinhonha e Mucuri, Rodovia MG 367, Km 583, Nº 5.000, Diamantina/MG Brasil

Abstract. *This work aims to study transient diffusion in solids with cylindrical shape. A numerical solution of the diffusion equation for this geometry is presented, for the boundary condition of the third kind. The one-dimensional diffusion equation was discretized using the finite volume method, with a fully implicit formulation. The solution can be used to simulate diffusive processes and to determine thermo-physical parameters, via optimization techniques. The developed package was applied to study the thin-layer drying of peeled bananas, using experimental data available in the literature. Three models were used to describe the drying process: 1) the volume V and the effective mass diffusivity D are considered constant; 2) variable V and constant D ; 3) V and D are considered variable. For all models, the convective mass transfer coefficient h is considered constant. The statistical indicators enable to conclude that model 3 describes the drying process much better than the other models.*

Keywords: *Optimization, Convective boundary condition, Diffusion model, Finite volume method, Numerical solution.*

1. INTRODUCTION

It is well known that to increase the post-harvest life of agricultural products, methods as cooling and drying, among other, should be used. For the drying case, many mechanisms as solar and hot air are available to accomplish the process. Moreover, in order to describe the drying process, generally a mathematical model is used.

Liquid diffusion models are used by several authors to describe the thin layer drying of foodstuffs (Phoungchandang and Wodds, 2000; Gastón et al., 2002; Lima et al., 2002; Doymaz, 2005; Amendola and Queiroz, 2007; Resende et al., 2007; Hacıhafızoglu et al., 2008; Silva et al., 2008). In order to use a diffusive model, the diffusion equation must be solved. If the geometry of the solid is simple and the shrinkage is neglected, in general an analytical solution can be obtained (Luikov, 1968; Crank, 1992). Moreover, if the effective diffusivity is supposed to be variable, as well as the volume of the solid, the diffusion equation should be numerically solved. Among the available methods, one commonly used is the finite volume method (Patankar, 1980; Silva et al., 2008). As example, Wu et al. (2004) used this method employing a fully implicit formulation to describe heat and mass transfer inside a single rice kernel during the drying process. In this work, the authors used generalized coordinates due to the irregular shape of the grain, and they considered the diffusivity and the volume as constant values. Another example of the use this method can be found in Lima et al. (2002). These authors used finite volume in order to describe the drying process of peeled bananas, coupling mass and heat transfer.

According to Baini and Langrish (2006) the world production of bananas is increasing almost every year. Banana is a typical fruit of wet tropical weather zones, being consumed mainly *in natura*. In countries as India (first producer) and Brazil (second producer), the product losses is approximately of 40%. In order to avoid losses, bananas are also consumed as “banana-passa”, which is the dried product. Several research works are found in the literature to describe drying of this product, using experimental data (Queiroz and Nebra, 2001; Lima et al., 2002; Karim and Hawlader, 2005; Amendola and Queiroz, 2007). In these works, several diffusion models considering analytical and numerical solutions are proposed to describe the drying process of peeled bananas, involving hypotheses with respect to the boundary conditions, shrinkage and effective mass diffusivity, among other. In this sense, it seems appropriate to examine what is the most adequate model to describe the drying process of this product.

This article uses a solution of the diffusion equation with the boundary condition of the third kind in order to compare models used to describe thin-layer drying of peeled bananas. To accomplish that, the diffusion equation was numerically solved through the finite volume method, using the fully implicit formulation. For the analyzed models, the effective mass diffusivity and convective mass transfer coefficient was determined via optimization, using the inverse method. After that, these parameters were used to simulate the drying process, and the best model was determined by the statistical indicators.

2. MATERIAL AND METHODS

The diffusion equation, many times used to describe water transport in porous media, can be written for an infinite cylinder as (Luikov 1968; Crank 1992):

$$\frac{\partial M}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left(r D \frac{\partial M}{\partial r} \right), \quad (1)$$

where M is the moisture content in dry basis, t is the time, r defines the radial position within the cylinder, and D is the effective water diffusivity.

In this paper, three diffusion models will be used in order to describe the drying of banana, supposing this product as an infinite cylinder submitted to the boundary condition of the third kind. The first model assumes constant volume and effective diffusivity. The second model supposes variable volume and constant effective diffusivity. Finally, the third model supposes variable volume and effective diffusivity.

In order to solve numerically the diffusion equation considering the three models above mentioned, the finite volume method (Patankar, 1980), was used with a fully implicit formulation. In this sense, the following hypotheses were assumed: 1) diffusion is the only transport mechanism of water inside the solid; 2) the solid is considered homogeneous and isotropic; 3) the convective mass transfer coefficient is constant during the water diffusion; 4) the diffusion process presents radial symmetry; 5) the characteristics of the drying air do not change during the whole process.

2.1. Numerical solution

Figure 1 presents a cylinder and its uniform grid. The control volumes have a thickness Δr and the control volume “i” has a nodal point “P”.

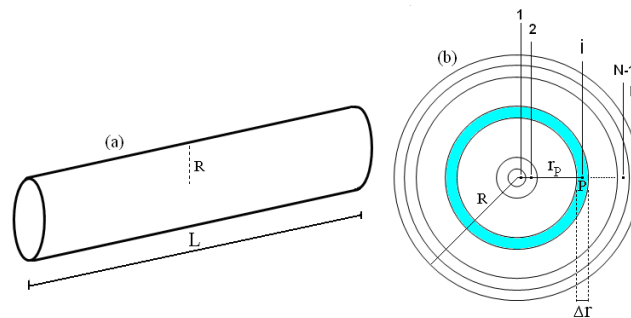


Figure 1. (a) Cylinder of radius R and height L ; (b) Uniform grid.

If the height L is much greater than the radius R and the radial symmetry exists, then Eq. (1) can be used to describe a drying process.

Figure 2 shows the control volume with nodal point “P” and its neighbors to west (W) and east (E). The lowercases “w” e “e” refer to the interfaces of the control volume “P”. On the other hand, r_w and r_e are the radius of the circumferences at the faces “w” and “e” of the control volume.

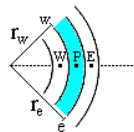


Figure 2. Control volume P and its neighbors to west (W) and east (E).

Using the finite volume method (Patankar, 1980) with the fully implicit formulation and integrating Eq. (1) on space ($2 \pi r_p \Delta r L$) and time (from t up to $t + \Delta t$), the following result is obtained for the control volume P:

$$\frac{M_P - M_P^0}{\Delta t} r_p \Delta r = r_e D_e \frac{\partial M}{\partial r} \Big|_e - r_w D_w \frac{\partial M}{\partial r} \Big|_w, \quad (2)$$

where the subscript 0 means “former time” and its absence means “current time”.

2.1.1. Internal Volumes

For the internal control volumes, the partial derivatives can be approximated as follows:

$$\left. \frac{\partial M}{\partial r} \right|_e \cong \frac{M_E - M_P}{\Delta r}, \quad (3)$$

and

$$\left. \frac{\partial M}{\partial r} \right|_w \cong \frac{M_P - M_W}{\Delta r}. \quad (4)$$

Thus, from Eq. (2), the discretized equation for an internal volume is written as follows:

$$A_w M_W + A_p M_P + A_e M_E = B, \quad (5)$$

where

$$A_w = -\frac{r_w \Delta r}{\Delta r} D_w; \quad A_p = \frac{r_p \Delta r}{\Delta t} + \frac{r_e}{\Delta r} D_e + \frac{r_w}{\Delta r} D_w; \quad (6a-d)$$

$$A_e = -\frac{r_e}{\Delta r} D_e; \quad B = \frac{r_p \Delta r}{\Delta t} M_P^0.$$

2.1.2. Control volume 1

For the control volume 1, due to the symmetry, the third term of Eq. (2) is zero. Then, the discretized equation becomes:

$$A_p M_P + A_e M_E = B, \quad (7)$$

with

$$A_p = \frac{r_p \Delta r}{\Delta t} + \frac{r_e}{\Delta r} D_e; \quad A_e = -\frac{r_e}{\Delta r} D_e; \quad (8a-c)$$

$$B = \frac{r_p \Delta r}{\Delta t} M_P^0.$$

2.1.3. Control volume N

For the control volume N, Eq. (3) is given in the following way:

$$\left. \frac{\partial M}{\partial r} \right|_e \cong \frac{M_b - M_P}{\Delta r / 2}, \quad (9)$$

where M_b is the value of M at the surface (boundary). On the other hand, the boundary condition of the third kind is expressed as

$$-D \left. \frac{\partial M}{\partial r} \right|_e = h(M_b - M_\infty), \quad (10)$$

in which M_∞ is the equilibrium moisture content (dry basis). Substituting Eq. (9) into Eq. (10), it is obtained:

$$D_e \frac{(M_b - M_p)}{\Delta r/2} = h(M_\infty - M_b). \quad (11)$$

Equation (11) can be used to express M_b as follows:

$$M_b = \frac{D_e M_p + \frac{h\Delta r}{2} M_\infty}{D_e + \frac{h\Delta r}{2}}. \quad (12)$$

Substituting Eq. (12) into Eq. (10) and the result into Eq. (2), the following expression is obtained for the discretized equation:

$$A_w M_w + A_p M_p = B, \quad (13)$$

where

$$A_w = -\frac{r_w \Delta r}{\Delta r} D_w; \quad A_p = \frac{r_p \Delta r}{\Delta t} + \frac{r_e D_e}{\frac{D_e}{h} + \frac{\Delta r}{2}} + \frac{r_w}{\Delta r} D_w; \quad (14a-c)$$

$$B = \frac{r_p \Delta r}{\Delta t} M_p^0 + \frac{r_e D_e}{\frac{D_e}{h} + \frac{\Delta r}{2}} M_\infty.$$

If the initial moisture content is known, then in each time step the system of equations given by Eq. (5), (7) and (13) can be solved, for instance, by the TDMA method (Press et al., 1996). If the radius of the cylinder varies, then, in each time step, its value must be calculated again, and also the thickness Δr .

Once $M(r,t)$ is numerically determined, the average value of moisture content at an instant t can be calculated through expression

$$\bar{M} = \frac{1}{V} \sum_{i=1}^N M_i V_i, \quad (15)$$

with

$$V = \sum_i^N V_i. \quad (16)$$

The aforementioned system of equations can be solved for the dimensionless moisture content, which is defined in the following way:

$$\bar{X}^* = \frac{\bar{M} - M_\infty}{M_0 - M_\infty}. \quad (17)$$

where the initial moisture content M_0 (dry basis) is supposed uniform. In this case, for $t = 0$, $\bar{X}^* = 1$ and for $t \rightarrow \infty$, $\bar{X}^* = 0$.

2.2 Effective mass diffusivity

For the nodal points, the effective mass diffusivity D can be calculated from an appropriate relation between such parameter and the local moisture content M ,

$$D = f(M, a, b), \quad (18)$$

where “ a ” and “ b ” are parameters which fit the numerical solution to the experimental data, and they can be determined by optimization.

On the interfaces of the control volumes, for example “ e ” (Fig. 2), the following expression should be used to determine D (Patankar, 1980; Silva et al., 2008):

$$D_e = \frac{2D_E D_P}{D_E + D_P}, \quad (19)$$

and Eq. (19) is valid for uniform grids. Note that Eq. (19) is also valid for a constant diffusivity, with a value D . In this case, $D_E = D$ and $D_P = D$; and Eq. (19) results in $D_e = D$ as expected. If the effective mass diffusivity is constant, the coefficients A of Eq. (5), (7) and (13) are calculated only once, and B is calculated in each time step because its value depends on M_P^0 , which is the value of M in the control volume P at the initial instant of each time step. On the other hand, if the parameter D is variable, the coefficients A are also calculated in each time step, due to the nonlinearities caused by the variation of such parameter. In this case, if the time refinement is adequate, errors due to the nonlinearities can be discarded.

2.3 Optimization

To determine the parameters D and h by optimization, the objective function was defined by the chi-square referring to the fit of the simulated curve to the experimental data of the drying kinetics. The expression for the chi-square involving the fit of a simulated curve to the experimental data is given by (Bevington and Robinson, 1992; Taylor, 1997)

$$\chi^2 = \sum_{i=1}^{N_p} \left(\overline{M}_i^{\text{exp}} - \overline{M}_i^{\text{sim}} \right)^2 \frac{1}{\sigma_i^2} \quad (20)$$

where $\overline{M}_i^{\text{exp}}$ is the average moisture content measured in the experimental point “ i ”, $\overline{M}_i^{\text{sim}}$ is the correspondent simulated average moisture content, N_p is the number of experimental points, $1/\sigma_i^2$ is the statistical weight referring to the point “ i ”. In general, in the absence of information, the statistical weights are made equal to 1. In Eq. (20), the chi-square depends on $\overline{M}_i^{\text{sim}}$, which depends on D and h . If the value of h can be considered constant and the thermal diffusivity is given by Eq. (18), the process parameters can be determined through the minimization of the objective function, which is accomplished in cycles involving the following steps:

- Step 1) Inform the initial values for the parameters “ a ”, “ b ” and “ h ”. Solve the diffusion equation and determine the chi-square;
- Step 2) Inform the value for the correction of “ h ”;
- Step 3) Correct the parameter “ h ”, maintaining the parameter “ a ” and “ b ” with constant values. Solve the diffusion equation and calculate the chi-square;
- Step 4) Compare the latest calculated value of the chi-square with the previous one. If the latest value is smaller, return to the step 2; otherwise, decrease the last correction of the value of “ h ” and proceed to step 5;
- Step 5) Inform the value for the correction of “ a ”;
- Step 6) Correct the parameter “ a ”, maintaining the parameters “ b ” and “ h ” with constant values. Solve the diffusion equation and calculate the chi-square;
- Step 7) Compare the latest calculated value of the chi-square with the previous one. If the latest value is smaller, return to the step 5; otherwise, decrease the last correction of the value of “ a ” and proceed to step 8;
- Step 8) Inform the value for the correction of “ b ”;

- Step 9) Correct the parameter “b”, maintaining the parameters “a” and “h” with constant values. Solve the diffusion equation and calculate the chi-square;
- Step 10) Compare the latest calculated value of the chi-square with the previous one. If the latest value is smaller, return to the step 8; otherwise, decrease the last correction of the value of “b” and proceed to step 11;
- Step 11) Begin a new cycle coming back to the step 2 until the stipulated convergence for the parameters “a”, “b” and “h” is reached.

In each cycle, the value of the correction of each parameter can be initially modest, compatible with the tolerance of convergence imposed to the problem. Then, for a given cycle, in each return to the step 2, 5 or 8, the value of the new correction can be multiplied by the factor 2. If the modest correction initially informed does not minimize the objective function, in the next cycle its value can be multiplied by the factor -1. Note that if the thermal diffusivity is supposed constant, the steps 8, 9 and 10 are not necessary. On the other hand, the initial values for the parameters can be estimated through obtained values for similar products available in the literature, or through some empirical correlation.

2.4 Developed software and statistical indicators

The developed software (optimizer and solver for the diffusion equation), including the user interface, was created in a computer Intel Pentium IV with 2 GB RAM; in the studio Compaq Visual Fortran Professional Edition V. 6.6.0, using a programming language option called QuickWin Application, under the Windows XP platform. Basically, the developed software can be used in two situations: 1) simulation of the cooling kinetics when the process parameters are known; 2) determination of the parameters D and h by optimization when an experimental dataset is known.

In order to analyze the quality of the fit, the statistical indicators chi-square, given by Eq. (20), and the coefficient of determination R^2 (Taylor, 1997) are used. All the statistical treatment of the obtained results is performed using the LAB Fit Curve Fitting Software, available on www.labfit.net.

2.5 Experimental data

The procedure proposed in this article for the determination of D and h was applied to the experimental data available in Queiroz and Nebra (2001), referent to the drying of banana *Musa acuminata* using hot air at the temperature of 29.9 °C. The general information about the drying process is given in Tab. 1.

Table 1. Information about the drying air (temperature T, relative humidity RH, and velocity v); moisture content of the bananas (initial, final and equilibrium); and drying time.

Air			Banana			t (h)
T (°C)	RH (%)	v (ms ⁻¹)	\overline{M}_o (db)	\overline{M}_f (db)	\overline{M}_∞ (db)	
29.9	35.7	0.38	3.43	0.32	0.1428	121.8

The data of dimensionless moisture content as function of the time have been obtained by digitizing the graph available in Queiroz and Nebra (2001), using the software xyExtract Graph Digitizer available at the internet in the link http://zeus.df.ufcg.edu.br/labfit/index_xyExtract.htm.

For the temperature of 29.9 °C, the radius R of the banana varies as function of the average dimensionless moisture content \overline{X}^* according the following expression:

$$R = 0.01613 (0.4981 + 0.5979 \overline{X}^*) \quad (21)$$

3. RESULTS AND DISCUSSION

3.1. Model 1: constant volume and effective mass diffusivity

In order to describe drying process using model 1 (constant volume and effective mass diffusivity), a grid with 100 control volumes was used, and the drying time was divided into 1000 steps. An unreported study about the grid and time refinement indicates that such values are adequate to describe the process. The results obtained by optimization are presented in Tab. 2 (SI).

Table 2. Results for the optimization process using model 1.

D (m^2s^{-1})	6.737×10^{-10}
h (ms^{-1})	9.175×10^{-8}
χ^2	1.229×10^{-3}
R^2	0.999525

Using the values of the parameters presented in Tab. 2, the drying process can be simulated, and the result is shown in Fig. 3 with the time given in hours.

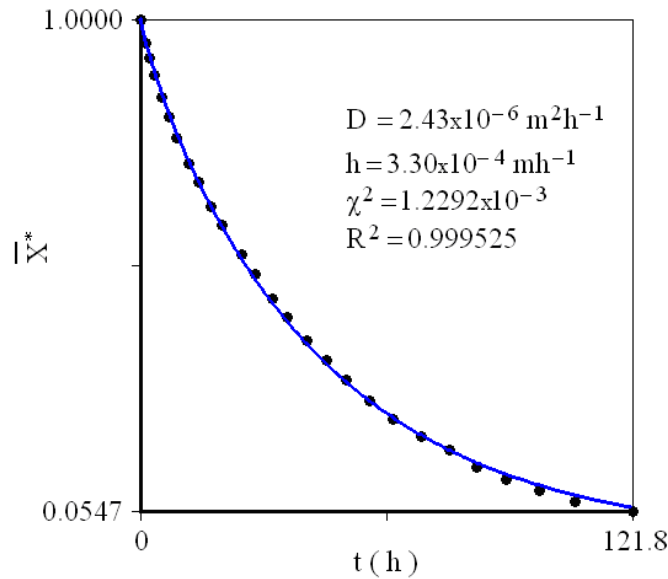


Figure 3. Drying kinetics of banana through model 1.

An inspection in Tab. 2 and Fig. 3 indicates that model 1 presents good statistical indicators. Thus, in an initial analysis, it can be conclude that the proposed model is good. However, despite the obtained good results, this model presents a fail: the shrinkage is not considered even being so expressive, as observed by Queiroz and Nebra (2001).

3.2. Model 2: Variable volume and constant effective mass diffusivity

For model 2 (variable volume and constant effective mass diffusivity), a grid with 100 control volumes was also used, and the drying time was also divided into 1000 steps. At the end of each time step, the radius was re-calculated using Eq. (21), and this new radius was used in the calculations of next time step. The results obtained by optimization are presented in Tab. 3 (SI).

Table 3. Results for the optimization process using model 2.

D (m^2s^{-1})	1.641×10^{-10}
h (ms^{-1})	2.115×10^{-7}
χ^2	4.8474×10^{-3}
R^2	0.998138

As it was made for model 1, using the values of the parameters presented in Tab. 3, the drying process can be simulated, and the result is shown in Fig. 4 with the time given in hours.

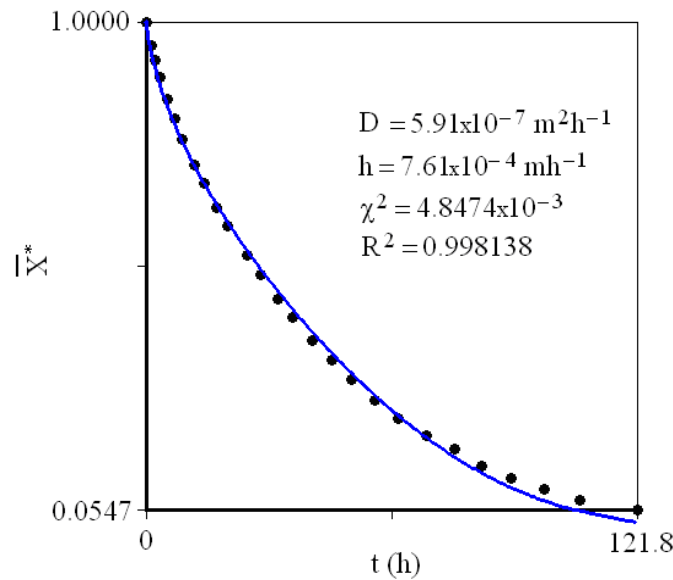


Figure 4. Drying kinetics of banana through model 2.

It is worth pointing out that, including the shrinkage effect, the obtained results are worst than those obtained disregarding this effect, if the effective mass diffusivity is supposed be constant in both cases.

3.3. Model 3: variable volume and effective mass diffusivity

For model 3 (variable volume and effective mass diffusivity), a grid with 100 control volumes was also used, and the drying time was divided into 2000 steps. In the end of each time step, the radius was re-calculated using Eq. (21), and this new radius was used in the calculations of next time step. Besides that, the coefficients A of Eq. (5), (7) and (13) was also re-calculated at the end of each time step seeking to minimize error due to the nonlinearities caused by the variation of the effective mass diffusivity, which influences such parameters. On the other hand, an inspection in Fig. 3 enables to assume that, at the final part of the drying process, the effective mass diffusivity should be less than the obtained value for model 2. It means that when the dimensionless average moisture content decreases, the effective mass diffusivity should also to decrease. The following expression for the effective mass diffusivity as function of the local dimensionless moisture content was proposed by Marinos–Kouris and Maroulis (1995):

$$D = b \exp(a X^*), \tag{22}$$

where a and b are constants that fit the numerical solution to the experimental data.

Equation (22) was used in the optimization of the drying process and the obtained results are presented in Tab. 4 (SI).

Table 4. Results for the optimization process using model 3.

D (m^2s^{-1})	$1.100 \times 10^{-10} \exp(1.690X^*)$
h (ms^{-1})	1.064×10^{-7}
χ^2	8.643×10^{-5}
R^2	0.999966

Using the values of the parameters presented in Tab. 4, the drying process can be simulated, and the result is shown in Fig. 5 with the time given in hours.

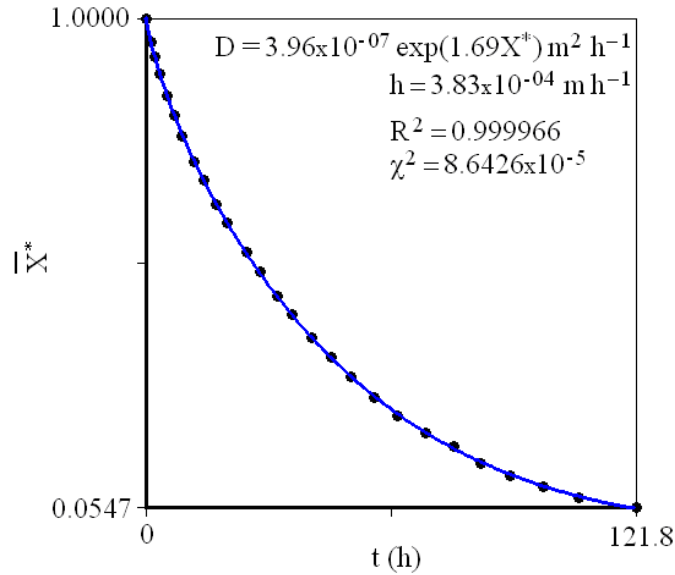


Figure 5. Drying kinetics of banana through model 3.

Once the drying parameters have been determined, Eq. (12) can be used in order to determine the dimensionless moisture content for each time step. The obtained results for model 3 are presented through Fig. 6.

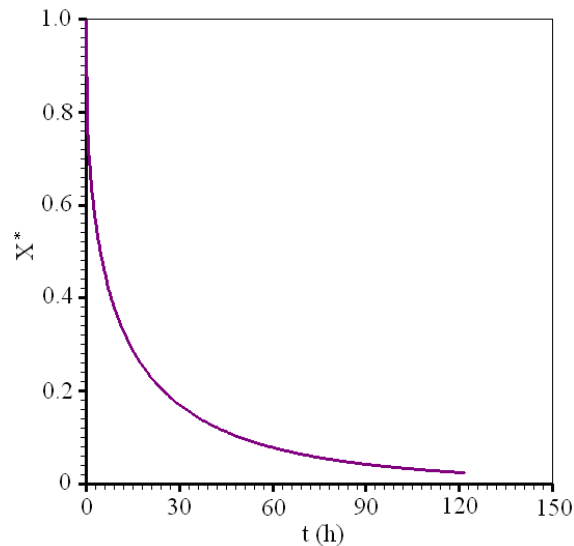


Figure 6. (a) Dimensionless moisture content at the boundary.

An inspection in Fig. 6 indicates that really the appropriate boundary condition to describe drying of bananas is of the third kind.

3.4. Discussion

Model 1 (constant volume and effective mass diffusivity) results in statistical indicators which can be considered good. However, this model does not consider the strong shrinkage. But when this effect was included (model 2), the statistical indicators become worst than previous one. Probably, the shrinkage also affects the effective moisture content due to the modifications within the internal structure of the bananas. Thus, It seems reasonable to assume that the two effects (shrink and changing in D) are mutually canceled. If this assumption is correct, the good results for model 1 are explained. Moreover, a model that includes the two effects should to yields better results than model 1. In fact, the chi-

square of model 1 is about 14 times greater than chi-square of model 3. In addition, the coefficient of determination of model 3 is 0.999966 while for model 1 is 0.999525.

Obviously, a larger number of parameters to express the effective mass diffusivity should improve the simulated result of the drying kinetics. But the objective of this paper has another focus: in some physical situations, such as drying of banana, the effective mass diffusivity with a value constant is inadequate to describe the drying kinetics. Some unreported expressions to express the effective mass diffusivity as function of the local dimensionless moisture content were also used in this research, but the best results were obtained through Eq. (22).

4. CONCLUSION

The simulation of the drying kinetics using model 1 presents good results, but this model does not consider the shrinkage. On the other hand, if the shrinkage is considered and the effective mass diffusivity is maintained with constant value (model 2), the results are worst than model 1.

The better model for the description of banana drying using hot air should include: 1) shrinkage, and 2) variable effective mass diffusivity, corresponding to model 3. The best result was obtained supposing an expression for the effective mass diffusivity, which increases with the local dimensionless moisture content. For the analyzed experimental data, the effective mass diffusivity is best represented by the exponential function. In this case, the chi-square is about 14 times less than the value obtained for model 1.

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6. RESPONSIBILITY NOTICE

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