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THE FINITE-VOLUME APPROACH FOR THE SOLUTION OF THE TRANSIENT DIFFUSION EQUATION APLLIED TO PROLATE SPHEROIDAL SOLIDS

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Abstract. *A numerical solution of the diffusion equation to describe heat or mass transport inside ellipsoids, considering variable diffusion coefficient and convective boundary condition is presented. The diffusion equation in prolate spheroidal coordinate system for a bidimensional case, was used. A finite volume method was employed to discretize the basic equation utilizing a uniform grid size. The equation was solved iteratively by the Gauss-Seidel method. To validate the numerical model, the results obtained were compared with the analytical solution. The model was used to solve the case of wheat grain drying, the results were compared with experimental data. This technique can be also applied in the processing of products with variable properties during different processes (drying, wetting, heating and cooling). The results show also that the model is consistent and it may be used to solve other cases, like those which include cylinder and sphere geometry and/or those with other boundary conditions, with small modifications.*

Keywords: *Prolate spheroids, Numerical, Diffusion, Drying, Variable properties*

1. INTRODUCTION

An intense research on mass transfer in solid or porous bodies has been done by various investigators. From the literature review, it is apparent that only very well known geometric bodies have been assumed to solve mass diffusion problems, specifically: parallelepipeds, cylinders and spheres. To get an analytical solution of a partial differential equation with a high level of complexity is sometimes difficult, in this case a numerical solution may be used to predict the phenomenon. Numerical studies of heat and mass diffusion in plate, cylinder and sphere are very well known (Crank ,1992; Gebhart 1993).

In this paper, a methodology of solution is presented for mass diffusion in bodies of elliptical shape. Previous studies about this subject can be found in Elvira (1990), Lima *et al.* (1997), Lima & Nebra (1997). The objective of this study is to describe numerically in 2-D case, the mass diffusion in the interior of prolate spheroidal solids. The model of liquid diffusion utilizing variable diffusion coefficient and convective boundary condition was used.

The mass diffusion equation in the prolate spheroidal coordinate system is presented and the finite volume method utilized to discretize this equation.

2. MATHEMATICAL FORMULATION

For the problem studied, the following considerations were made:

- Shrinkage of the body is neglected;
- the phenomenon occurs under falling rate;
- the solid is assumed to be homogeneous;
- thermophysical properties were assumed to be dependent of moisture content
- the body is axi-symmetrical around z-axis;

Under the above conditions, assuming that the moisture content gradient is the driving force of the drying process, the Fick's second law of diffusion has been used by a number of investigators. It is also admitted that liquid diffusion is the only mechanism of moisture movement. The mass diffusion equation in cartesian coordinate system is given by (Strumillo and Kudra, 1986):

$$\frac{\partial M}{\partial t} = \nabla \cdot \left(D \nabla M \right) \tag{1}$$

where D is the diffusion coefficient, M is the moisture content and t, is the time.

In many physical problems it is better to use an orthogonal coordinate system ξ, η, ζ instead of the cartesian coordinate x, y, z. The choice of a particular coordinate system is motivated by the geometrical form of the body in study, and can result in a considerably simplified analysis of the problem. In the case of a body with elliptical geometric form, an adequate coordinate system is the prolate spheroidal coordinate system. The relations between cartesian and prolate spheroidal coordinate system are given by (Magnus *et al.*,1966):

$$x = L\sqrt{(1-\xi^2)(\eta^2-1)}\ \zeta \qquad y = L\sqrt{(1-\xi^2)(\eta^2-1)}\ \sqrt{(1-\zeta^2)} \qquad z = L\xi\eta \tag{2}$$

where ξ=coshμ; η=cosϕ, ζ =cosω and $L=(L_2^2 - L_1^2)^{1/2}$, is the focal length. The domain of the variables ξ, η and ζ with relation the Figure 1 is given by: $1 \leq \xi \leq L_2/L$; $0 \leq \eta \leq 1$ and $0 \leq \omega \leq 2\pi$.

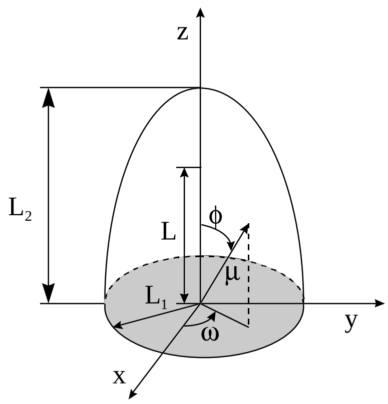

Figure 1- Characteristics of the prolate spheroidal solid

The surfaces $\xi=\xi_o$ (constant) are ellipsoids of revolution around z-axis and $\eta=\eta_o$ (cte) are hyperboloids of two sheets. The surfaces $\omega=\omega_o$ (cte) are planes through z-axis. Calculating the metrical coefficients and with the use of the expression for the Laplacian in prolate spheroidal coordinate system (Abramowitz & Stegun, 1972) we obtain the mass diffusion equation in prolate spheroidal coordinate system, Equation (3).

$$\frac{\partial M}{\partial t}=\left[\frac{1}{L^2\left(\xi^2-\eta^2\right)}\frac{\partial}{\partial \xi}\left(D\left(\xi^2-1\right)\frac{\partial M}{\partial \xi}\right)\right]+\left[\frac{1}{L^2\left(\xi^2-\eta^2\right)}\frac{\partial}{\partial \eta}\left(D\left(1-\eta^2\right)\frac{\partial M}{\partial \eta}\right)\right]+ \\ +\frac{\sqrt{1-\zeta^2}}{L^2\left(\xi^2-1\right)\left(1-\eta^2\right)}\frac{\partial}{\partial \zeta}\left(D\sqrt{1-\zeta^2}\frac{\partial M}{\partial \zeta}\right) \quad (3)$$

Admitting symmetry around the z axis, $\partial/\partial\omega=0 \Rightarrow \partial/\partial\zeta=0$, the Equation (3) can be written as follows:

$$\frac{\partial M}{\partial t}=\left[\frac{1}{L^2\left(\xi^2-\eta^2\right)}\frac{\partial}{\partial \xi}\left(D\left(\xi^2-1\right)\frac{\partial M}{\partial \xi}\right)\right]+\left[\frac{1}{L^2\left(\xi^2-\eta^2\right)}\frac{\partial}{\partial \eta}\left(D\left(1-\eta^2\right)\frac{\partial M}{\partial \eta}\right)\right] \quad (4)$$

with the following boundary conditions:

- Free surface: the diffusive flux is equal to the convective flux at the surface of the prolate spheroid

$$\frac{D}{L}\sqrt{\frac{\left(\xi^2-1\right)}{\left(\xi^2-\eta^2\right)}}\frac{\partial M}{\partial \xi}\bigg|_{\xi=\xi f}+h_m\left[M\left(\xi=\xi_f,\eta,t\right)-M_e\right]=0$$ with $\xi_f=L_2/L$ in the surface.

where h_m is the mass transfer coefficient and M_e, the equilibrium moisture content.

- Planes of symmetry: the angular and radial gradients of moisture content are equal to zero at the planes of symmetry.

$$\frac{\partial M(\xi;1;t)}{\partial \eta}=0 \qquad \frac{\partial M(\xi;0;t)}{\partial \eta}=0 \qquad \frac{\partial M(1;\eta;t)}{\partial \xi}=0$$

- Constant initial conditions in the interior of the solid

$M(\xi;\ \eta;\ 0)=M_o$ = cte

The average moisture content of the body was calculated as follows (Whitaker, 1980):

$$\overline{M}=\frac{1}{V}\int_V M dV \quad (5)$$

Then,

$$\overline{M}=\frac{1}{\int_0^1\int_1^{\frac{L2}{L}}\left(\xi^2-\eta^2\right)d\xi d\eta}\int_0^1\int_1^{\frac{L2}{L}}M(\xi,\eta)\left(\xi^2-\eta^2\right)d\xi d\eta \quad (6)$$

In these equations, V is the total volume in the domain considered for the new coordinate system, calculated according Magnus *et al.* (1966).

3. NUMERICAL FORMULATION

Due to the symmetry existing in the body, the computational domain showed in Figure 2 was adopted, where the nodal points (P, N, S, W, E) are also presented.

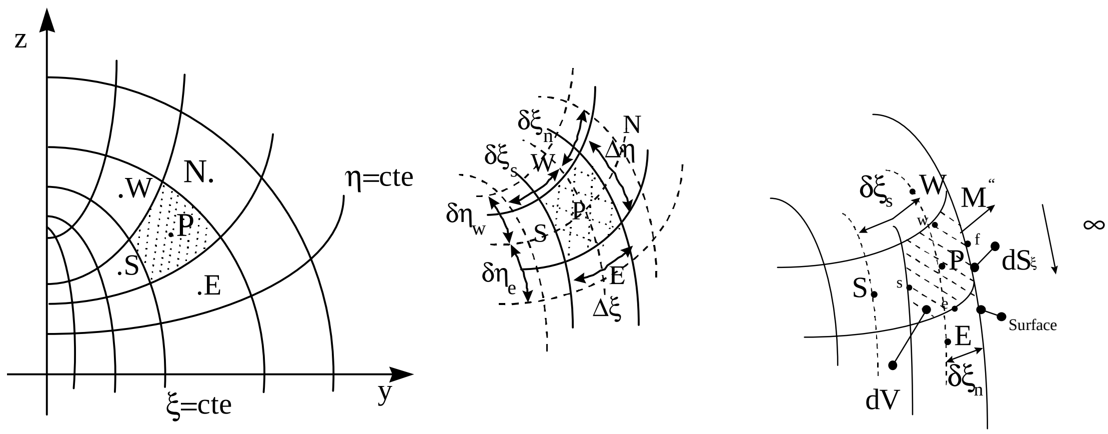

Figure 2- Geometrical configuration of the physical problem.

Equation (4) was discretized by a finite-volume method utilizing the practice B (the nodal points are located in the center of the control-volume) (Patankar, 1980 and Maliska, 1995) in a uniform grid size. The discretized equation is given below:

$$A_P M_P = A_N M_N + A_S M_S + A_E M_E + A_W M_W + A_P^o M_P^o \tag{7}$$

where:

$$A_N = \frac{D_n(\xi_n^2 - 1)\Delta\eta}{\delta\xi_n} \qquad A_S = \frac{D_s(\xi_s^2 - 1)\Delta\eta}{\delta\xi_s} \qquad A_E = \frac{D_e(1-\eta_e^2)\Delta\xi}{\delta\eta_e}$$

$$A_W = \frac{D_w(1-\eta_w^2)\Delta\xi}{\delta\eta_w} \qquad A_P^o = \frac{\Delta\xi\Delta\eta L^2(\xi_P^2 - \eta_P^2)}{\Delta t} \qquad A_P = \sum A_K + A_P^o + S$$

$$S = \frac{\Delta\eta}{\left[\dfrac{D_p}{h_m L\sqrt{\left[(\xi_f)^2 - (\eta_P)^2\right]}\sqrt{\left[(\xi_f)^2 - 1\right]}} + \dfrac{\delta\xi_n}{\left[(\xi_f)^2 - 1\right]}\right]}$$

The coefficients A_K, $K \neq P$, reflect the contributions of the diffusive transport of M, from the neighbor nodes in direction to the node P. The quantity S is a source term, it contains the moisture content at the surface that is added to the nodal points preceding the boundary points. Only in these nodal points the coefficient A_N is equal to zero. For the other nodal points S is equal to zero and A_N is given by the expression presented above.

Considering that the interface i is placed in the midway between P and I, then D_i can be expressed by:

$$D_i = \frac{2D_P D_I}{D_P + D_I} \tag{8}$$

where i represents the interface e, w, n and s.

With known values of M from the immediately preceding solution of the Eq. (7), the set of equations was solved iteratively using the fully implicit scheme by the Gauss-Seidel method. The calculation was done utilizing a uniform grid size 20 x 20 points and time interval Δt=20s. The results of the moisture content are independent of the grid and time step (Lima *et al.*, 1997). The calculation starts with the given initial condition and stopped when the following convergence criteria were satisfied in each point of the computational domain:

$$\left|M^{*n+1} - M^{*n}\right| \leq 10^{-8} \qquad \frac{\sum\left|A_K\right|}{\left|A_P\right|} \leq 1 \text{ for all equations.} \tag{9}$$

where n represent the n th iteration in each step time.

4. APLICATIONS

In order to test the formulation presented in this work, two different examples were analyzed: Transient mass diffusion within a spherical body and the wheat grain drying (variety AVALON). A computational code called SPHEROIDIFF utilizing the Microsoft Fortran Power Station was written to solve the set of equations for the moisture content profile and to determine the average moisture content for the cases studied.

4.1 Diffusion in spherical solid with convection at surface

The first example analyzed was that of a solid sphere at initial condition $M^*=(M-M_e)/(M_o-M_e)=1.0$ and subjected to the following boundary condition $Bi=h_mL/D_p=1.0$, where Bi is the Biot number of mass transfer. In this case, the physical properties were assumed to remain constant ($D_e=D_w=D_n=D_e=D_p$=constant), in this case the numerical model can be treated with dimensionless variables (Lima & Nebra, 1998).

The analytical solution is available from the literature and actual values were obtained by summing the twenty first terms of the infinite series.

As a comment, the exact solution of the diffusion in prolate spheroidal solids subjected to convection at surface is not reported in the literature.

4.2 Wheat kernel drying

In this example, the wheat drying experimental data presented by Fioreze (1986) through thin-layer drying equation, were used. The air drying conditions were: temperature, T=55 ^{o}C and relative humidity, RH=6,2%. For the wheat grain we have M_o=0.3350 (d.b.) and M_e=0.0480 (d.b.). Using linear regression technique, Fioreze (1986) determined the following thin-layer drying equation:

$$\overline{M}^{*} = \frac{\overline{M} - M_e}{M_o - M_e} = \text{Exp}\left(-0.8418\, t^{0.5582}\right) \tag{10}$$

where t is given in hours, according to the author, the comparison between the predicted and the experimental data presents an average error of 0.13%. The characteristic data of wheat utilized in the simulation were (Brooker *et al.*, 1992): L_1=0.0015748m and L_2=0.0032760 m. The quantity M_o is the initial moisture content of the grain.

In his study Fioreze (1986) presented a diffusion coefficient as a function of the moisture content and the temperature obtained by the comparison of the experimental and numerical data, considering wheat grain as sphere and Fickian diffusion. This equation is presented as follows:

$$D = \overline{M}^{a_1}\,\text{Exp}\left(a_2\overline{M} + a_3\right) \tag{11}$$

with a_1=-2.85554.10^{-5}T+1.6432; a_2=0.4113T-30.2634; a_3=-2.2776.10^{-2}T-9.7271 and D given in m^2/h. In this equation T is given by in ^{o}C.

In the present numerical method wheat grain is considered as na ellipsoid, then it was necessary to fit the Eq. (11) for the present case multiplying it by a constant a_o.

The diffusion and mass transfer coefficients were found by varying the D and h_m to minimize the sum of squared deviations between the actual and predicted data. The relative deviation between experimental and calculated values (relative residuals, ERMQ) and the variance (S^2) are defined as follows:

$$E = \sum_{i=1}^{n}\left(\overline{M}^{*}_{i,Num} - \overline{M}^{*}_{i,Exp}\right)^2$$

$$S^2 = \frac{E}{(n-1)} \tag{12}$$

where n is the number of experimental points (Carnahan *et al.*, 1969).

The smallest values of E and S^2 were used as a criteria to obtain the best value of the diffusion coefficient D and mass transfer coefficient.

5. RESULTS AND DISCUSSIONS

5.1 Example 1

To validate the numerical model, results of this work were compared with analytical results for sphere (L_2/L_1=1.0), with Bi=1.0 (Luikov, 1966). The Figure 3 illustrates the comparison of the concentration ratio obtained numerically in this work with the analytical solution with twenty terms of the series, for a sphere, as a function of radial position inside the solid for divers Fourier numbers, defined this time as Dt/R^2 ($R=L_1=L_2$). As it may be observed, quasi-complete concordance exists between the results.

Similar agreement was obtained comparing the average concentrations during the process.

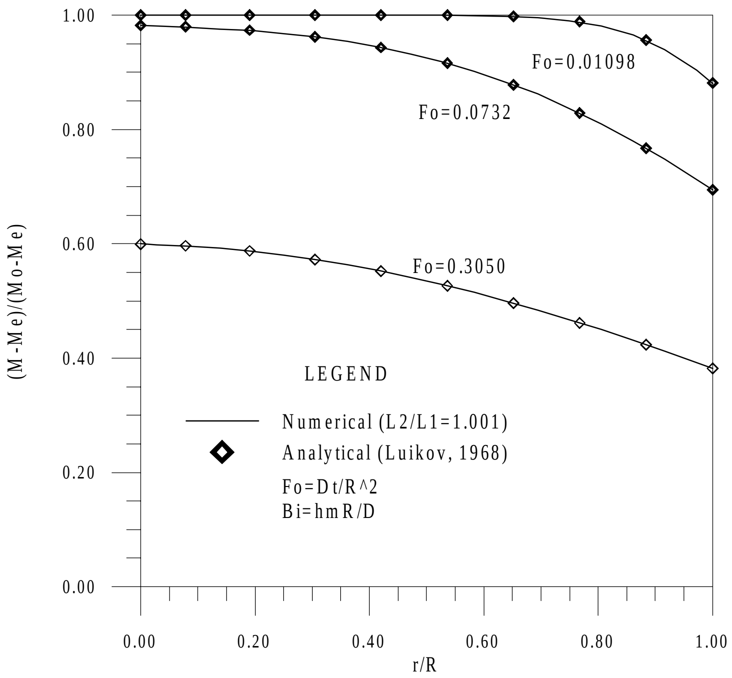

Figure 3 - Comparison between the concentration ratio inside of a sphere (L_2/L_1=1.0) and Bi=1.0, obtained by the numerical method, proposed by the authors and the analytical method (Luikov, 1968)

5.2 Example 2

Figure 4 shows the wheat with its respective numerical grid generated. It must be observed that the shape of the mesh varies with L_2/L_1, when $L_2/L_1 \to \infty$, the focal point is dislocated to the surface of the body, the inverse occurs for $L_2/L_1 \to 1$, when the focal point tends to be coincident with the geometrical center of the body.

Observe that on z-y plane, the control-volumes are not uniformly spaced, presenting a great concentration near the surface of the body, relative to ξ (radial coordinate), and the y axis relative to η (angular coordinate). That characterizes a non-regular grid; however, in the $\xi\eta$ plane, we have a regular grid. This grid has the property that the ratio of lengths of any two adjacent intervals is a constant and equal to one. In this plane are performed all the numerical calculations.

The diffusion coefficient and mass transfer coefficient were estimated using experimental data and admitting that the best fitted value is obtained when the smallest value of E, defined by Eq. (12), is found. The diffusion and mass transfer coefficients found, were:

$$D = 0.55\overline{M}^{a_1}\mathrm{Exp}\left(a_2\overline{M} + a_3\right) \qquad h_m = 15.44.10^{-7}\ \mathrm{m/s}$$

These results showed that the difference between the diffusion coefficient obtained considering the wheat like a sphere and like a prolate spheroid is 45%. This is very significant.

Figure 5 illustrates the comparison between numerical and predicted values of average moisture content of wheat during drying process. The curve indicates the accuracy with which the diffusion theory could predict drying behavior. A good agreement can be observed. The error in the estimation of the diffusion coefficient D, is 0.72% and variance 0.0124% .

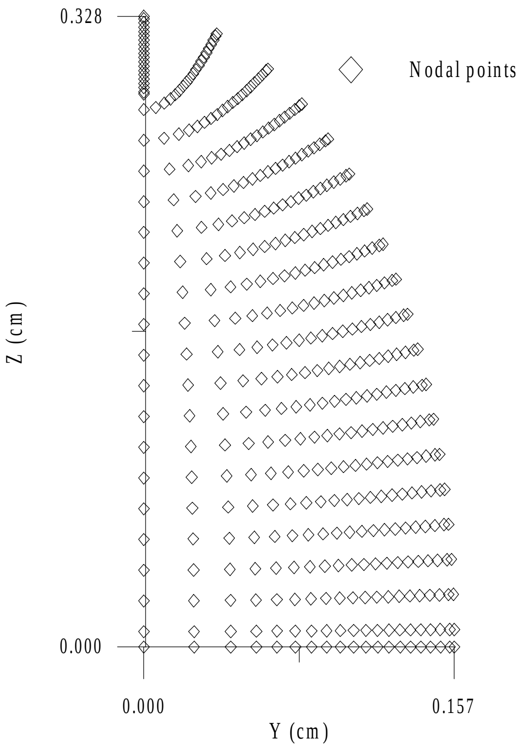

Figure 4 - Numerical grid in the physical plane for the example 2.

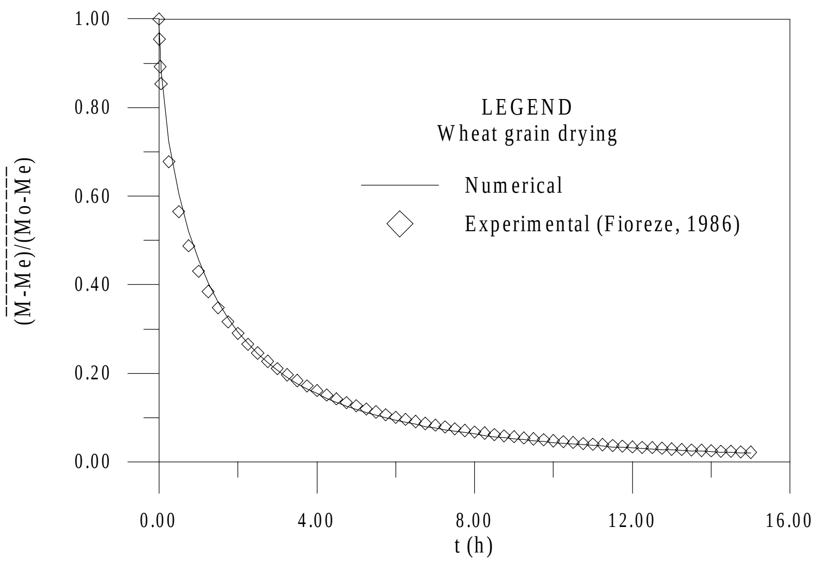

Figure 5 - Predicted and experimental values of dimensionless average moisture content during thin-layer drying of wheat grain at T= 55^{o}C and RH=6.2%

Figure 6 shows the effect of drying time on the moisture content distribution inside the wheat grain. The iso-concentration lines, which represent surfaces in the space, are shown. It can be seen that the difference between the moisture content in the center and focal point is very great. This is due to the localization of the focal point. These results indicate that mass diffusion occurs initially faster in the exterior region of the solid, decreasing with the drying time in direction to the center of the solid.

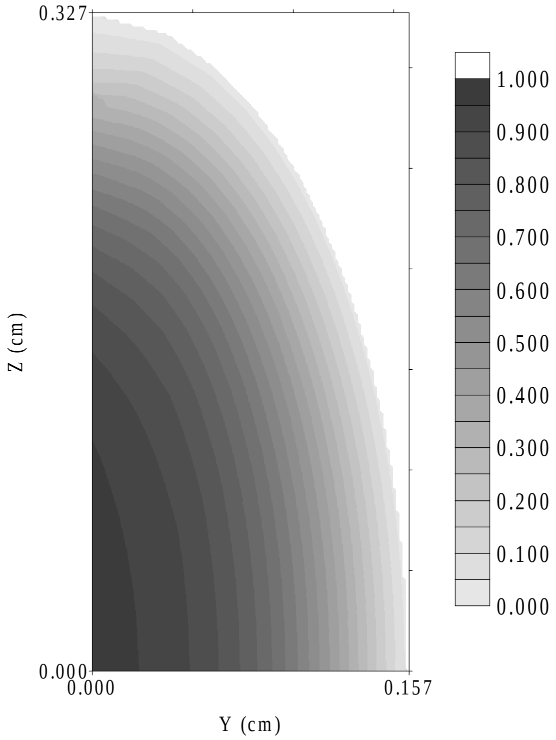

Figure 6 - The distribution of the moisture content and the iso-concentration lines inside of wheat grain in t=1.11 h

The numerical results also indicate that the dependence of the moisture content with the angular coordinate η, is very strong. The concentration ratio decreases faster in the extremity of the z axis ($z=L_2$), decreasing this effect to the end of y axis ($z=L_1$). This behavior is due to the geometrical form of the body.

6. CONCLUSIONS

The finite volume formulation for the diffusion in prolate spheroid bodies with variable properties was presented. From the examples shown, it can be concluded that this formulation is accurate and it is efficient to simulate many practical problems of diffusion such as heating, cooling, wetting and drying, particularly in prolate spheroids, but it can be used for spheres also. This formulation is useful also with material variable properties, when there is no an analytical solution and in cases including other boundary conditions, with small modifications.

REFERENCES

Abramowitz, M. & Stegun, I. A., 1972, Handbook of mathematical functions, Dover Public., Inc., New York, pp. 752-772

Brooker, D. B.; Bakker-Arkema, F.W. & Hall, C.W., 1992, Drying and storage of grains and oilseeds, AVI Book, New York.

Crank, J., 1992, The mathematics of diffusion, Oxford Science Publications, New York.

Elvira, C. de, 1990, Diffusion process modeling in elliptic shaped bodies, Proceedings of the 6th International Congress of Engineering and Food,. London, vol. 1, pp. 456-464.

Fioreze, R., 1986, The intermittent drying agricultural crops with particular reference to energy requeriments. Ph. D Thesis, Granfield Institute of Technology, Silsoe College.

Gebhart, B., 1993, Heat conduction and mass diffusion, McGraw-Hill, Inc., New York.

Lima, A. G. B., Nebra, S. A. & Altemani, C. A. C., 1997. Simulation of the drying kinetics of the silkworm cocoon considering diffusive mechanism in elliptical coordinate, Proceedings of the Inter-American Drying Conference, July, Itu, Volume B, pp. 317-324.

Lima, A. G. B.; Nebra, S. A., 1997, Influência de parâmetros geométricos na cinética de secagem de elipsóides sólidos, XXV Congresso Brasileiro de Sistemas Particulados (XXV ENEMP), Outubro, São Carlos. v.1, pp. 195-202

Luikov, A.V., 1968, Analytical heat diffusion theory, Academic Press, Inc.Ltd., London.

Magnus, W.; Oberhettinger, F.; Soni, R. P., 1966, Formulas and theorems for the special functions of mathematical physics, Springer-Verlag, Berlim, pp. 472-495.

Maliska,C.R.,1995,Transferência de calor e mecânica dos fluidos computacional, LTC, Rio de Janeiro.

Patankar, S.V.,1980, Numerical heat transfer and fluid flow, Hemisphere Publish. Coop, New York.

Strumillo, C.; Kudra, T., 1986, Drying: principles, science and design, Gordon and Breach Science Publishers, New York.

Whitaker, S., 1980, Heat and mass transfer in granular porous media, Chapter Two, in Advances in drying, ed. Arun S. Mujumdar, Hemisphere Publishing Corporation, Volume 1, New York.