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ANALYTICAL SOLUTION OF THE MASS DIFFUSION EQUATION APPLIED TO ELLIPSOIDS OF REVOLUTION

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Abstract. *The mathematical solution of the transient diffusion equation is very important, especially on drying operations, where it is necessary to know the moisture content distribution, and also the average moisture content of biological products in function of position and time. The derivation of an analytical solution of the mass diffusion equation in prolate spheroidal coordinates, assuming constant diffusion coefficient for products with elliptical geometry, is presented. The moisture content distribution and also the average moisture content during the process are shown. This solution can be used to predict the behavior of the drying process during the drying of a given type of product, varying the characteristic parameters, and also to validate numerical resolution of the same differential equation in elliptical geometry.*

Keywords: *Analytical, Diffusion, Drying, Ellipsoid, Spheroid*

1. INTRODUCTION

The analytical solution of the diffusion equation has been obtained for various boundary conditions with constant or variable diffusion coefficient, in homogeneous or heterogeneous and isotropic or anysotropic bodies, and in steady or non steady-state cases. The partial differential equation for non steady-state mass diffusion has been solved for mass transfer in bodies with single geometry, as plates, cylinders and spheres with specified boundary conditions (Luikov, 1968, Skelland, 1974 and Crank, 1992).

The non steady-state diffusion solutions are very important especially in drying process where it is necessary to know the moisture content distribution like inside biological products. A lot of biological products has the form of prolate spheroids, cereals, fruits, it seems that this form is the "natural form in the nature".

Haji-Sheikh & Sparrow (1966) gave an analytical solution of the heat transfer equation in a prolate spheroidal body with constant temperature at the surface using an elliptical coordinate system in bidimensional case.

The objective of this work is to develop an analytical solution to describe the moisture transport in a continuous medium, utilizing the elliptical coordinate system in bidimensional case. The moisture content distribution in the product and the average moisture content in each time step for bodies with elliptical geometry, will be also obtained.

2. MASS DIFFUSION EQUATION IN THE PROLATE SPHEROIDAL COORDINATE SYSTEM

Newman & Sherwood, cited by Bakshi & Singh (1980), proposed the application of Fick's law for the drying of solids during the decreasing ratio of drying process. This mass diffusion equation is given by:

$$\frac{\partial M}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial M}{\partial x}\right) + \frac{\partial}{\partial y}\left(D\frac{\partial M}{\partial y}\right) + \frac{\partial}{\partial z}\left(D\frac{\partial M}{\partial z}\right) \qquad (1)$$

where D is mass diffusion coefficient and M is the moisture content of the product in each instant of time t.

Depending on the geometrical form of the body, a coordinate system, adequate to describe the domain in study, must be selected. In the specific case of ellipsoid of revolution, the adequate one is the prolate spheroidal system. The relations between the cartesian (x, y, z) and prolate spheroidal (μ, ϕ, ω) coordinate systems are given by Haji-Sheikh & Sparrow (1966):

$$x = L \sinh\mu.\sin\phi.\cos\omega \qquad y = L \sinh\mu.\sin\phi.\sin\omega \qquad z = L\cosh\mu.\cos\phi \qquad (2)$$

where L is the focal length equal to $(L_2^2 - L_1^2)^{1/2}$. The scheme of an ellipsoid of revolution is shown in Figure 1.

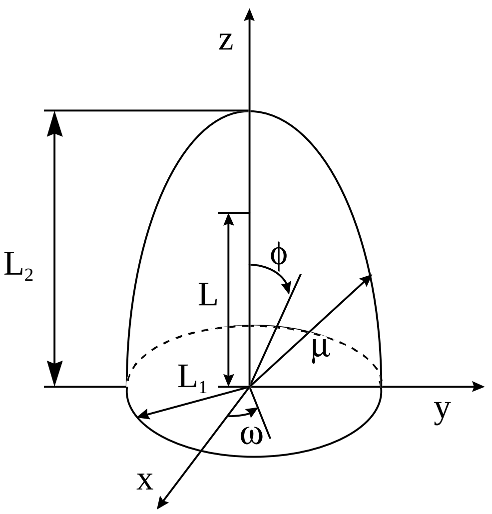

Figure 1- Characteristics of an ellipsoid of revolution solid

Defining ξ=cosh μ, η=cos ϕ and ζ= cos ω, the metrics coefficient and the Laplacian to the new coordinate system can be obtained using the mathematical relations given by Abramowitz & Stegun (1972). Utilizing the metrics coefficients, the variables ξ, η and ζ and the differentiation's rules, the transient mass diffusion equation is given by:

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

For a situation with symmetry around the z axis, is:

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

When the initial moisture content distribution in the interior of the solid is uniform and constant in the surface at all time, the boundary conditions of Eq. (4) are:

$M(\xi,\eta,0)=M_o$ = constant; $M(\xi,\eta,t)= M_e$ = constant (at surface) (5)

The method of solution used in this work is the separation of variables, assuming that $M(\xi,\eta,t)=\psi(\xi,\eta)\theta(t)$. The solution of Eq. (4) is then, (Haji-Sheikh & Sparrow, 1966):

$$M=\psi(\xi,\eta)\exp(-c^2Dt/L^2) \tag{6}$$

Assuming a constant D, applying the Eq. (6) to Eq. (4), we have:

$$\left(\frac{-c^2}{L^2}\right)\psi=\frac{1}{L^2(\xi^2-\eta^2)}\left[\frac{\partial}{\partial\xi}\left((\xi^2-1)\frac{\partial\psi}{\partial\xi}\right)\right]+\frac{1}{L^2(\xi^2-\eta^2)}\left[\frac{\partial}{\partial\eta}\left((1-\eta^2)\frac{\partial\psi}{\partial\eta}\right)\right] \tag{7}$$

which can be written in a short form:

$$\nabla^2\psi+\left(\frac{c^2}{L^2}\right)\psi=0 \tag{8}$$

Assuming that we can separate variables as $\psi(\xi,\eta)=\chi(\xi).\lambda(\eta)$, putting it into Eq. (8), and separating the variables, two ordinary differential equation are obtained:

$$\left[\frac{d}{d\xi}\left((1-\xi^2)\frac{d\chi}{d\xi}\right)\right]+(b-c^2\xi^2)\chi=0 \tag{9}$$

$$\left[\frac{d}{d\eta}\left((1-\eta^2)\frac{d\lambda}{d\eta}\right)\right]+(b-c^2\eta^2)\lambda=0 \tag{10}$$

In Equations (9) and (10), b is the separation constant or eigenvalues. These two equations are exactly in the same form, λ as a function of η, varies between 0 and the singular point +1, while χ as a function of ξ, varies between the singular point +1 and L_2/L. The solution of the angular function $\lambda(\eta)$ is expressed in terms of a Legendre function series of the first kind, while $\chi(\xi)$ is obtained of a spherical Bessel functions series of the first kind of order n. The solution of the Eqs. (9) and (10) are given by:

$$\chi_m(c,\xi)=\left[\sum_{n=0}^{\infty}d_{n,m}\right]^{-1}.\sum_{n=0}^{\infty}(-1)^{\frac{n-m}{2}}.d_{n,m}j_n(c\xi);\quad \lambda_m(c,\eta)=\sum_{n=0}^{\infty}d_{n,m}(c).P_n(\eta) \tag{11}$$

with m=0,2,4,... and n=0,2,4,... . Utilizing the recurrence relations (Flammer, 1957), the successive coefficients $d_{n,m}$ are obtained.

$$\alpha_r d_{r+2,m} + (\beta_r - b_n) d_{r,m} + \gamma_r d_{r-2,m} = 0 \qquad (12)$$

where:

$$\alpha_r = \frac{(r+2)(r+1)c^2}{(2r+5)(2r+3)}; \quad \beta_r = \frac{[(2r)(r+1)-1]c^2}{(2r-1)(2r+3)} + r(r+1); \quad \gamma_r = \frac{r(r-1)c^2}{(2r-3)(2r-1)}$$

with r=0, 2, 4... . The b_n values are given by the transcendental equations below:

$$U(b_n) = U_1(b_n) + U_2(b_n) = 0 \qquad (13)$$

with

$$U_1(b_n) = \varphi_n - b_n - \cfrac{\delta_n}{(\varphi_{n-2} - b_n) - \cfrac{\delta_{n-2}}{(\varphi_{n-4} - b_n) - \ \dots}}; \qquad (14)$$

$$U_2(b_n) = -\cfrac{\delta_{n+2}}{(\varphi_{n+2} - b_n) - \cfrac{\delta_{n+4}}{(\varphi_{n+4} - b_n) - \ \dots}} \qquad (15)$$

and

$$\delta_n = \frac{n^2(n-1)^2 c^4}{(2n-1)^2(2n+1)(2n-3)}; \quad n \geq 2 \qquad \varphi_n = n(n+1) + \frac{c^2}{2}\left[1 + \frac{1}{(2n-1)(2n+3)}\right]; \quad n \geq 0$$

The technique utilized to determine the b_n coefficients is denominated continued fraction technique (Stratton *et al.*, 1956). This technique has been used to determine the eigenvalues to c≤8.0. When c≥10.0, the eigenvalues are obtained through an asymptotic expansion. The asymptotic development of b_n is given by the successive approximations method, as follows:

$$\begin{aligned} b_n = {} & (2n+1)c - \frac{(2n^2+2n+3)}{2^2} - \frac{(2n+1)(n^2+n-3)}{2^4 c} - \frac{5(n^4+2n^3+7n+3)}{2^6 c^2} - \\ & - \frac{(66n^5+165n^4+962n^3+1278n^2+1321n+453)}{2^{10}c^3} - \\ & - \frac{(252n^6+75n^5+5885n^4+10510n^3+18478n^2+13349n+4425)}{2^{12}c^4} - \\ & - \frac{[527(2n+1)^7+61529(2n+1)^5+1043961(2n+1)^3+2241599(2n+1)]}{2^{20}c^5} + O(c^{-6}) \end{aligned} \qquad (16)$$

A convergent series for $d_{n,m}$ may be obtained for a discrete set of values of the eigenvalues b_n. There are two sets of finite solutions, one for even values of n, the other for odd values. The lowest value of b_n corresponds to n=0, the next to n=2, and so on (Morse & Feshbach, 1953), so the set corresponding to even values of n was used in this work. The values of the coefficients $d_{n,m}$ are different, depending on the normalization scheme adopted. The criterion utilized by the authors is presented below:

$$\sum_{r=0}^{\infty} \frac{(-1)^{r/2}(r)!}{2^r\left(\frac{r}{2}\right)!\left(\frac{r}{2}\right)!} d_{r,m} = \frac{(-1)^{n/2}(n)!}{2^n\left(\frac{n}{2}\right)!\left(\frac{n}{2}\right)!} \qquad (17)$$

for r=0,2,... and n=0,2,... .

The Equation (17) together with (16) or (12), allows the complete determination of the coefficients $d_{n,m}$. The index n is in all of the cases ≥0. For n<0 we have $P_n(\eta)=0$ indicating that the series really begin at n=0.

The condition that restricts the values of the b_n in the differential equations is reflected in Eq. (12) as a requirement that the ratio of the coefficients $d_{n,m}/d_{n-2,m}\rightarrow 0$, when $n\rightarrow\infty$ (Stratton *et al.*,1956). Observing that the coefficients c, b and d must be obtained satisfying $\chi_m=0$ in the surface of the prolate spheroidal ($\xi=L_2/L$).

With the coefficients $d_{n,m}$ determined, the general solution of the problem studied is given by:

$$M(\xi,\eta,t)-M_e=\sum_{m=0,2}^{\infty}\sum_{k=1}^{\infty}A_{mk}e^{-c_{mk}^2\frac{Dt}{L^2}}\chi_m(c_{mk},\xi)\lambda_m(c_{mk},\eta) \tag{18}$$

The coefficients A_{mk} are obtained from the orthogonality conditions. Substituting the initial condition (5) in Eq. (18), it is obtained:

$$M_o-M_e=\sum_{m=0,2}^{\infty}\sum_{k=1}^{\infty}A_{mk}\chi_m(c_{mk},\xi)\lambda_m(c_{mk},\eta) \tag{19}$$

Multiplying both sides of Eq. (19) by $\chi_p(c_{pk},\xi)\lambda_p(c_{pk},\eta)(\xi^2-\eta^2)$ and integrating in a quarter of the volume of the ellipsoid, we obtain:

$$\begin{aligned}&\int_0^1\int_1^{L_2/L}\chi_p(c_{pk},\xi)\lambda_p(c_{pk},\eta)(\xi^2-\eta^2)(M_o-M_e)d\xi d\eta=\\&=\sum_{m=0,2}^{\infty}\sum_{k=1}^{\infty}\int_0^1\int_1^{L_2/L}\chi_p(c_{pk},\xi)\lambda_p(c_{pk},\eta)(\xi^2-\eta^2)A_{mk}\chi_m(c_{mk},\xi)\lambda_m(c_{mk},\eta)d\xi d\eta\end{aligned} \tag{20}$$

where the integration and the sum operations were exchanged.

Admitting that the integration in Eq. (20) can be made term by term, and considering the orthogonality of the functions, the only term in the right-hand side that supply an integral different from zero, is the term with m=p. For m=p, the results is:

$$A_{mk}=\frac{\int_0^1\int_1^{L_2/L}\chi_m(c_{mk},\xi)\lambda_m(c_{mk},\eta)(\xi^2-\eta^2)(M_o-M_e)d\xi d\eta}{\int_0^1\int_1^{L_2/L}\left[\chi_m(c_{mk},\xi)\lambda_m(c_{mk},\eta)\right]^2(\xi^2-\eta^2)d\xi d\eta} \tag{21}$$

where the denominator is the norm of $(\chi_m\ \lambda_m)(\xi^2-\eta^2)$. For the case where (Mo-Me) is a constant value, this term can be isolated of the integral and, moreover, the solution presented in Eq. (18) will become referred to moisture content ratio (M-Me)/(Mo-Me) instead of (M-Me).

Since M= M(ξ,η,t), the average moisture content of the solid can be calculated as follows:

$$\overline{M}=\frac{\int_0^1\int_1^{\frac{L_2}{L}}\left\{\sum_{m=0,2}^{\infty}\sum_{k=1}^{\infty}\left[\frac{A_{mk}}{(M_o-M_e)}\right]e^{-c_{mk}^2\frac{Dt}{L^2}}\chi_m(c_{mk},\xi)\lambda_m(c_{mk},\eta)\right\}(\xi^2-\eta^2)d\xi d\eta}{\int_0^1\int_1^{\frac{L_2}{L}}(\xi^2-\eta^2)d\xi d\eta} \tag{22}$$

considering the symmetry around z-axis.

3. RESULTS AND DISCUSSIONS

To get the moisture content ratio of a product as a function of the position and time, various results have been generated for a 2-D system. Two groups of results are of interest: the first concerning the drying kinetics and the second the moisture content profile variation inside the product along with the drying time. Table 1 presents for the aspect ratio $L_2/L_1=1.1$, the c values, roots of the radial spheroidal function χ, for $\xi=L_2/L$, the eigenvalues b of the expansion coefficients $d_{n,m}$, of the coefficients $A_{m.k}$ and finally, the values obtained for the orthogonality criteria for radial and angular functions. The choice of this aspect ratio to be related with the possibility of comparison of the mean moisture content obtained for this geometry with that for a sphere.

To obtain the values of the coefficients c, b and $d_{n,m}$ of the final solution presented in the Eq. (18), three computational programs were implemented utilizing the software Fortran Power Station; while to determine the coefficients $A_{m,k}$ and the orthogonality conditions of the function, two computational programs were implemented, utilizing the software Mathematica®. It can be observed that obtaining this analytical solution requires a lot of hard work and an excessive number of hours of computational work, comparing with the numerical solution given by Lima *et al.,* (1997). Some results obtained with the computational programs for given condition were exhaustively compared with the results supplied in the works of Flammer (1957), Haji-Sheikh & Sparrow (1966), Stratton *et al.* (1941), and Abramowitz & Stegun (1972). In particular, with relation to the results presented by Haji-Sheikh & Sparrow (1966) some differences were found, but, the deviations found do not modify the accuracy of the solution. These deviations have been produced by the number of terms utilized to obtain the $d_{n,m}$. In this work r = n = 0,2,...,30 and $\chi_m \leq 10^{-6}$ in $\xi=L_2/L$ (that correspond to the surface of the body) were used. The values given in the Table 1 may be used to reproduce the results shown in this work and to help investigators to validate computational codes in future works.

To validate the mathematical model, results of this work were compared with analytical results for an ellipsoid ($L_2/L_1=1.1$), with Bi infinite given by Haji-Sheikh &Sparrow (1966). Figure 2 shows the comparison between the concentration ratio in the center and focal point of a prolate spheroid as a function of Fo defined as $Fo=Dt/L_1^2$.

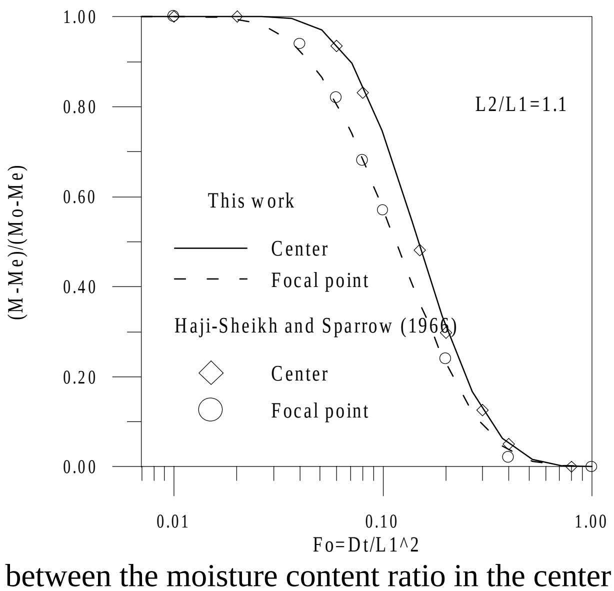

Figure 2 - Comparison between the moisture content ratio in the center and focal point of a spheroid with $L_2/L_1=1.1$, given by the authors and Haji-Sheikh &Sparrow (1966)

As may be observed, almost complete concordance exists between the results. Within the knowledge of the authors, no analytical solution was presented for the case of finite convective transfer coefficient.

Table 1. Values of the coefficients and orthogonality criterion of the spheroidal functions for $L_2/L_1=1.1$

m	k	c	b	$A_{mk}/(Mo - Me)$	$\int_0^1\int_1^{L_2/L}\chi_m\lambda_m\chi_p\lambda_p(\xi^2-\eta^2)d\xi d\eta$, $m\neq p$
0	1	1.397161	0.597864	2.20921	7.31×10^{-5}
	2	2.810801	1.941011	-2.56547	8.19×10^{-6}
	3	4.239071	3.417864	2.74925	-3.25×10^{-7}
	4	5.673506	4.878233	-2.82125	3.81×10^{-8}
	5	7.110252	6.327193	2.85634	-5.63×10^{-8}
	6	14.415977	13.677683	4.24925	4.29×10^{-5}
	7	15.730222	14.991063	-6.64284	1.03×10^{-4}
2	1	2.498990	9.546556	0.93749	7.31×10^{-5}
	2	3.939209	15.029440	-1.46940	-2.89×10^{-6}
	3	5.350201	21.975240	1.91801	1.02×10^{-6}
	4	6.767435	29.354480	-2.25566	6.01×10^{-7}
	5	11.213435	52.182143	1.34006	1.79×10^{-5}
	6	14.277787	67.545189	-1.44475	2.58×10^{-5}
	7	17.027654	81.314800	-3.85214	1.15×10^{-4}
4	1	3.560427	26.723961	0.20851	-5.65×10^{-5}
	2	5.080160	34.387491	-0.65941	-7.44×10^{-6}
	3	6.511387	44.760996	1.12838	-4.96×10^{-6}
	4	7.661939	74.551175	0.40166	6.33×10^{-6}
	5	12.215065	98.015325	1.81058	-3.31×10^{-5}
	6	13.697456	111.542129	-1.56309	-3.47×10^{-5}
	7	19.623852	165.259385	4.19315	1.11×10^{-4}
6	1	4.578694	52.897881	-0.07087	-1.05×10^{-4}
	2	6.179835	62.422934	-0.17630	1.29×10^{-6}
	3	13.324302	147.588863	1.85300	3.57×10^{-5}
	4	14.756208	166.798766	-1.78276	-1.90×10^{-6}
	5	16.212916	186.179002	1.56258	-1.75×10^{-5}
	6	17.712867	206.024129	-1.19208	1.33×10^{-5}
	7	20.776639	246.348095	0.93516	4.61×10^{-5}
8	1	7.244554	99.597313	-0.03961	-1.25×10^{-5}
	2	15.893173	225.716049	-1.69836	4.24×10^{-5}
	3	17.313937	250.899657	1.78127	7.65×10^{-6}
	4	18.754075	276.179925	-1.66311	-6.38×10^{-6}
	5	20.226143	301.844828	1.35443	-3.82×10^{-6}
10	1	18.469751	319.065393	1.87432	6.00×10^{-5}
	2	21.311389	381.524835	1.55890	-9.07×10^{-7}
	3	22.766709	413.099241	-1.42828	-6.11×10^{-6}
12	1	21.051540	427.609452	-1.46840	7.30×10^{-5}
	2	23.877066	502.122386	-1.56875	1.59×10^{-6}
14	1	26.448771	637.942151	1.35442	-5.44×10^{-6}

Figure 3 shows the analytical data of the moisture content profile as a function of the radial coordinate ξ, for a Fourier number defined as $Fo=Dt/L^2= 0.0089$. In this figure the data are plotted for three different angular position. The comparison of the curves indicate that for increasing values of η, the moisture content decrease for any ξ at any Fo. For increasing values of Fo, the moisture content profile decrease in any point (ξ, η), indicating that the moisture flux occurs from center in direction to the surface. The strong dependence of moisture content profile with the radial coordinate can also be observed, the profile is decreasing with the increase of ξ, for all values of Fo. This result is verified mainly for small Fourier numbers, where the moisture content gradients are high, except for the regions near the center of the body.

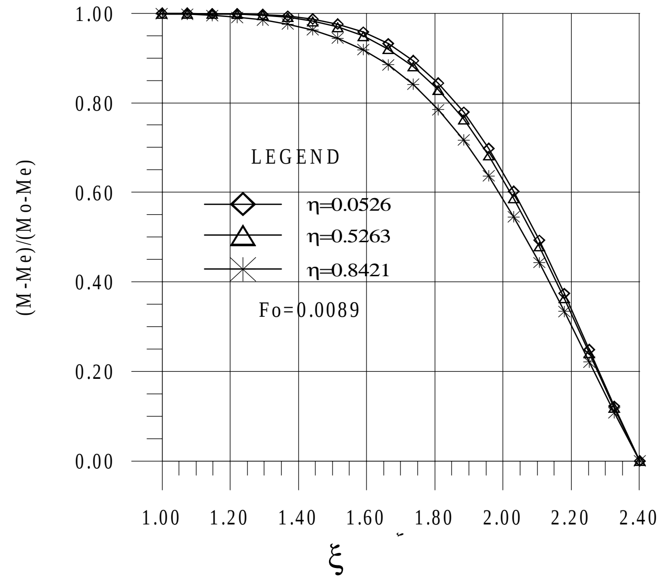

Figure 3- Profile of moisture content inside the prolate spheroid as a function of ξ, $L_2/L_1=1.1$

Figure 4 shows the shape of the moisture content profile in function of η for constant ξ and Fo. The analysis of the plots indicates that the profile decreases lightly with the angular coordinate for constant Fo at any ξ, mainly for small values of Fo and regions near the surface. This behavior is different from a sphere, where symmetry exists relative to the angular coordinate: in the case we are presenting, we have the geometrical condition $L_2/L_1=1.1$, which for a sphere is $L_2/L_1=1.0$. This difference will increase with increasing L_2/L_1.

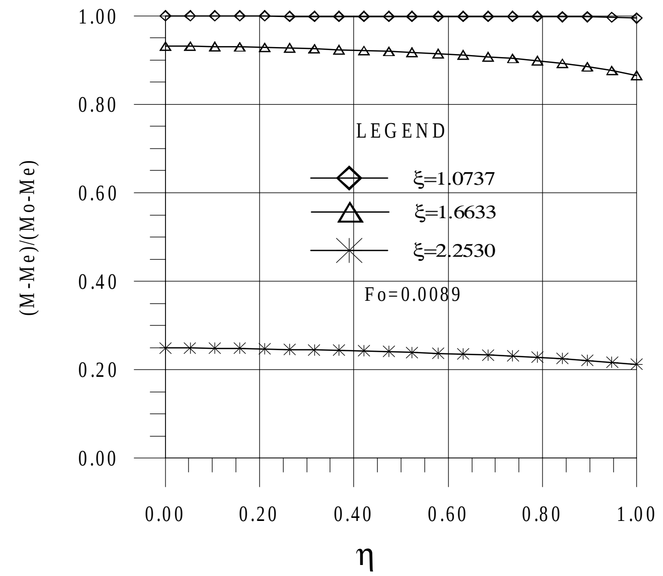

Figure 4- Profile of moisture content inside the prolate spheroid as a function of η ($L_2/L_1=1.1$)

Figure 5 shows the moisture content developed inside of the prolate spheroid, in the center, focal point and near the surface during the drying stage for various Fo. Some results are noted: the moisture content strongly depends on the Fo; the equilibrium moisture content is achieved at Fo≥4.0; the variation with the time of the moisture content profile are higher in the center of body in comparison with their behavior in the focal points and finally the moisture content profile is higher in the center of body then in the focal point, for any Fo. These results indicates that the equilibrium occurs first in the focal point going to the direction of the center with the increase of Fourier number.

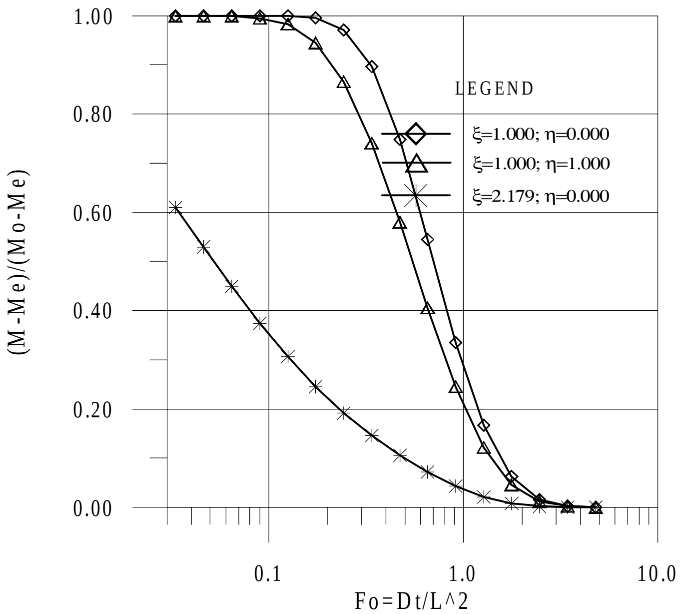

Figure 5- Moisture content in the center, focal point and near the surface for various Fo, $L_2/L_1=1.1$

The average moisture content, for three different geometries is shown in Figure 6, as a function of the Fourier number, here defined as Dt/L_1^2. Note that for this Fourier number the equilibrium moisture content is achieved at for Fo=1.00. The values for ellipsoid were calculated with Eq. (22), and for sphere and finite cylinder with the equations presented by Luikov (1968).

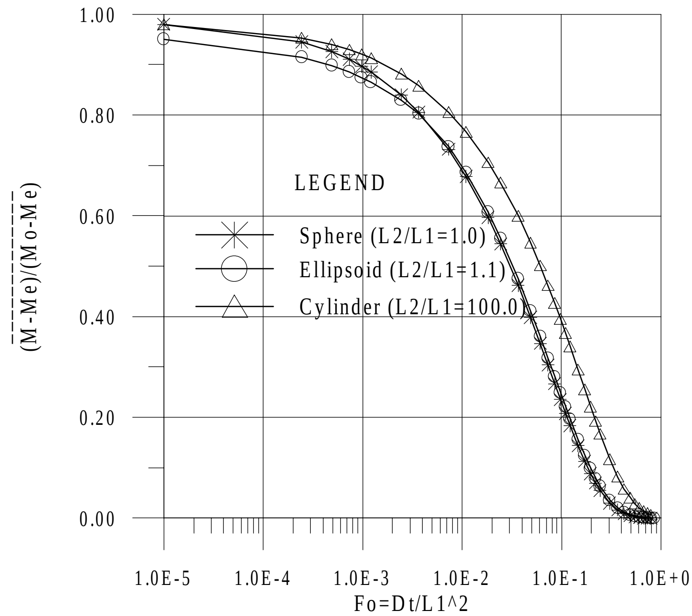

Figure 6 - Average concentration as a function of Fourier number, comparison between sphere, cylinder and ellipsoid.

As can be seen, the results for ellipsoid, calculated with the coefficients shown in Table 1, presents a small error for Fourier number lower than 0.004. This difference can be attributed to the instability of the Bessel functions for small Fourier numbers, and also to the successive approximations of .the method here presented, this last problem can be solved using a higher number of terms in the determination of the coefficients. For Fourier numbers higher than 0.005, the coefficients of Table 1 and Eq. (22) can be used to get average moisture content in ellipsoidal bodies without discrepancies. It is observed that the drying kinetics obtained for a prolate spheroidal solid with aspect ratio $L_2/L_1=1.1$ it is very close of that obtained for a sphere.

4. CONCLUSIONS

The analytical solution presented here can be used to obtain the moisture content distribution in the product and the average moisture content in each time step for bodies with elliptical geometry. The mean value of moisture content is particularly useful when the model is used to determine the diffusion coefficient from experimental data of drying kinetic. As the solution obtained is only referred to the case with equilibrium at the surface, it can be used to validate numerical solutions which can be extended to cases with less restrictive boundary conditions.

The dimensionless coordinates used, moisture ratio and Fourier number, were adequate to get general results, to be applied to any case. It can be say that for the mass diffusion as sole mechanism of moisture migration the moisture content distribution depends strongly of the radial coordinate and slightly of the angular coordinate, for Fo constant and an aspect ratio of $L_2/L_1=1.1$. The moisture content is strongly influenced by the Fo number in any position in the interior of the spheroid. The equilibrium moisture content is approached, at any point in the body, for $Fo=Dt/L^2 \geq 4.0$ ($L_2/L_1=1.1$).

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