NUMERICAL STUDY OF THE SIMULTANEOUS HEAT AND MASS TRANSFER IN PROLATE SPHEROIDAL BODIES BASED ON THE NON-EQUILIBRIUM THERMODYNAMICS

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Abstract. *A new mathematical modeling to describe simultaneous heat and mass (liquid and vapor) transfer in capillary-porous bodies with particular reference to prolate spheroid is presented. The mathematical model was based on the non-equilibrium thermodynamics considering variable transport coefficients and equilibrium boundary conditions at the surface of the solid. All the partial differential equations presented in the model have been written in prolate spheroidal coordinates. The finite-volume method was used to obtain the numerical solution of the problem using implicit fully formulation. Results of the average moisture content, and moisture content and temperature distributions in a wheat kernel during drying process are presented and analyzed. On the other hand, the methodology allows verifying the heat, liquid and vapor fluxes, taking into account the thermal and hydrical gradients inside the solid.*

Keywords*: drying, numerical solution, mass, diffusion, elliptical geometry*

1. Introduction

The diffusion phenomenon exists in many industrial applications such as drying, wetting, heating and cooling of biological products and principally foodstuffs (grains, fruits, vegetables, etc). From a review of the literature, it is noted that several researches prefer to diffusion model applied only to known geometric shapes specifically: parallelepipeds, cylinders, spheres (Skelland, 1974; Crank, 1992; Gebhart, 1993) and for prolate and oblate spheroidal bodies (Lima and Nebra 2000; Carmo and Lima, 2001; Lima and Nebra, 2001; Oliveira and Lima, 2002; Lima *et al.*, 2004;) with specified boundary conditions and constant thermo-physical properties Assuming moisture migration inside the solid by liquid or vapor diffusion only (Mikhailov and Shishedjiev, 1975; Luikov, 1975, Ribeiro *et al.*, 1993; Irudayaraj and Wu, 1996). However, other researchers shown that the moisture migrates in the liquid and vapor phases, due to concentration gradients, partial vapor-pressure gradients, capillary forces, differences in total pressure, gravity (Luikov and Mikhailov, 1965, Luikov, 1966; Mikhailov and Shishedjiev, 1975; Luikov, 1975, Fortes, 1978; Fortes and Okos, 1980; Fortes and Okos, 1981; Whitaker, 1980, Fortes e Okos, 1981; Ribeiro *et al.*, 1993; Irudayara and Wu, 1996). According to Luikov (1966), transfer of vapor and inert gas can take place by molecular means in the form of diffusion and by molar means by a filtration motion of the whole steam-gas mixture within the porous body under the influence of a fall in aggregate pressure. Therefore, the derivation of the rubs of mass transfer in a system of capillary-porous bodies on the basis of molecular and molar transfer mechanism presents great difficulties. In this sense, Fortes (1978) and Fortes and Okos (1981), Fortes *et al.*, (1981) presents a set of transport equations that incorporates most of the models presented in the literature by combining the mechanistic and irreversible thermodynamics approaches to heat and mass transfer in porous media. According to Fortes and Okos (1981) all the physical parameters cited in the model can be obtained from experimental techniques. The other side, many biological products has shape approximately ellipsoidal, in the particular case, prolate spheroidal. For examples, rice, wheat, orange, silkworm cocoon and banana. The problem of the heat and mass transfer in a prolate spheroid it is of great interest because, it represents a high degree of precision of the problem in comparison to the approach this problem for cases of sphere or cylinder as used today. Since that sphere and cylinder are particular cases of prolate spheroids, it is now unnecessary to repeat the complex derivation for each different geometric shape. How complement for these researches, in this paper, a two-dimensional numerical analysis is performed for simultaneous heat and mass (liquid and vapor) transport in bodies of ellipsoidal shape, using the Fortes and Oko's Theory (irreversible thermodynamic approaches) and the finite-volume technique to discretize the basic equations.

2. Models development

Consider the diffusion phenomenon in an ellipsoid of revolution, in which the axis of revolution is greater than the other axis as pictured in Figure 1. In this case it is said to be prolate, while, if the axis of revolution is smaller than the other, it is called oblate. As a simplification for the problem studied, the following considerations were made: The shape of solid is approached to an ellipsoid of revolution; The shrinkage is neglected; The unique mechanism of drying is diffusion; The solid is composed of water in liquid and vapor phases and solid material; Thermo-physical properties variables during drying process; The body is axially symmetric around z-axis; The moisture content and temperature field is considered symmetric around z-axis in any time and constant in the beginning of the process; The phenomenon occurs under equilibrium condition at the surface; No energy and mass generation occurs; Moisture migration (liquid and vapor) due to gravity is neglected; The diffusion phenomenon occurs under falling rate. In many physical problems it is better to use a new orthogonal coordinate system ξ,η,ζ instead of the Cartesian coordinate x, y, z. In the case of the body with ellipsoidal geometric shape, an adequate coordinate system is the prolate spheroidal coordinate system. The relation between Cartesian and prolate spheroidal coordinate systems are given by (Magnus *et al.*, 1966):

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

where $\xi=\cosh\mu$; $\eta=\cos\phi$; $\zeta=\cos\omega$ and $L=(L_2^2 - L_1^2)^{1/2}$.

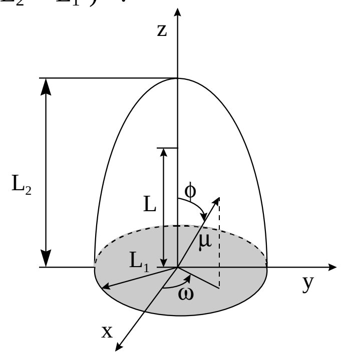

Figure 1. Geometrical parameters of a prolate spheroidal solid

2.1. Mass transfer

To mass transfer model $\Phi = M$ we have the following equations:

- Liquid flux:

$$\vec{J}_\ell = -\rho_\ell k_\ell R_v \ell nH\,\nabla T - \rho_\ell k_\ell \frac{R_v T}{H}\frac{\partial H}{\partial M}\nabla M + \rho_\ell k_\ell \vec{g} \tag{2}$$

- Vapor flux:

$$\vec{J}_v = -k_v\left(\rho_{vo}\frac{\partial H}{\partial T} + H\frac{d\rho_{vo}}{dT}\right)\nabla T - k_v\rho_{vo}\frac{\partial H}{\partial M}\nabla M + \left(\frac{Hk_v\rho_{vo}}{TR_v}\right)\vec{g} \tag{3}$$

where M should be taken as the equilibrium moisture content in any location inside the porous media. In this equations $\vec{g}$ is the gravitational acceleration vector; H is the relative humidity; k_l is the liquid conductivity; k_v is the vapor conductivity; M, Local moisture content; R_V is the universal gas constant as applied to air; T is the air temperature; ρ is the density.

Assuming that no ice is present, and that the mass of air is neglected, and that mass of vapor is neglected in relation to mass of liquid (but not its flux) (Luikov, 1966), a mass balance in an differential control volume leads to:

$$\frac{\partial(\rho_s M)}{\partial t} = -\nabla\cdot\left(\vec{J}_\ell + \vec{J}_v\right) \tag{4a}$$

with the following boundary conditions:

Free surface: the mass diffusive flux is equal to the mass convective flux at the surface of the solid.

$$M(\xi = \xi_f, \eta, t) = M_e \text{ with } \xi_f=L_2/L \text{ in the surface} \tag{4b}$$

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

$$\frac{\partial M(\xi;1;t)}{\partial\eta} = 0 \qquad \frac{\partial M(\xi;0;t)}{\partial\eta} = 0 \qquad \frac{\partial M(1;\eta;t)}{\partial\xi} = 0 \tag{4c-e}$$

Initial condition in the interior of the solid

$$M(\xi;\eta;0)=M_o \tag{4f}$$

The average moisture content of the body was calculated as follows:

$$\overline{M} = \frac{1}{V}\int_V M\,dV \tag{5}$$

2.2. Heat transfer

To heat transfer process, the transient heat conduction equation will be given by:

$$\frac{\partial}{\partial t}(\rho_s c_b T) - \frac{\partial}{\partial t}(\rho_s L_w M) = -\nabla.\vec{J}_q - \nabla.(L_v \vec{J}_v) - \vec{J}_\ell.c_\ell \nabla T - \vec{J}_v.c_v \nabla T \tag{6a}$$

where the c is the specific heat; h_c is the heat transfer coefficient. The flux vapor is given by:

$$\vec{J}_q = -k_T \nabla T - \left(\rho_\ell k_\ell R_v \ell nH + k_v\left(\rho_{v0}\frac{\partial H}{\partial T} + H\frac{d\rho_{v0}}{dT}\right)\right)\frac{R_v T^2}{H}\frac{\partial H}{\partial M}\nabla M + + T\left(\rho_\ell k_\ell R_v \ell nH + k_v\left(\rho_{v0}\frac{\partial H}{\partial T} + H\frac{d\rho_{v0}}{dT}\right)\right)\vec{g} \tag{6b}$$

where k_T is the thermal conductivity. More details about the notation may be found in the references cited in the text.

The boundary conditions are:

Free surface: the heat convective flux supplied to the body surface equals to the heat diffusive flux sum the energy necessary to evaporate the liquid water and to heat the vapor produced at the surface of the prolate spheroid from surface temperature to the air drying temperature.

$$\theta(\xi = \xi_f, \eta, t) = \theta_e \tag{6c}$$

Planes of symmetry: the angular and radial gradients of temperature are equals to zero at the planes of symmetry.

$$\frac{\partial\theta(\xi;1;t)}{\partial\eta} = 0 \qquad \frac{\partial\theta(\xi;0;t)}{\partial\eta} = 0 \qquad \frac{\partial\theta(1;\eta;t)}{\partial\xi} = 0 \tag{6d-f}$$

Initial condition inside the solid

$$\theta(\xi;\eta;0) = \theta_o \tag{6g}$$

The average temperature of the body during diffusion phenomenon was calculated as follows:

$$\bar{\theta} = \frac{1}{V}\int_V \theta\, dV \tag{7}$$

All equations were written in prolate spheroidal coordinate.

3. Numerical solution

3.1. Solution technique

Various numerical methods have been used to solve the problem of transient diffusion, such as, finite-difference, finite-element, and boundary element and finite-volume methods. Several discussions may be encountered in previous reports (Brebia and Domiguez, 1989; Patankar, 1980 and Maliska, 2004). In particular, in this work, the numerical method used was the finite-volume method. In the simulation of diffusion phenomenon in prolate spheroids was utilized a certain domain, due to the symmetry of the body. Assuming fully implicit formulation, the Equations 4a and 6a were integrated in the volume and time. How results the following dicretization equation was obtained:

$$A_P\Phi_P = A_E\Phi_E + A_W\Phi_W + A_N\Phi_N + A_S\Phi_S + A_P^0\Phi_P^0 + b \tag{8}$$

where Φ represents M or T.

3.2. Application to drying of wheat grain

The following expressions were used in the numerical simulation:

⇒ Saturated vapor density: $\rho_{vo} = (2.54 \times 10^8 / T)\exp(-5200/T)$ (kg/m^3) (Fortes *et al.*, 1981)

⇒ Water density: $\rho_l = 1000$ kg / m^3 (Fortes *et al.*, 1981)

⇒ Dry solid density: $\rho_s = 1265$ kg / m^3 (Fortes *et al.*, 1981)

⇒ Heat of vaporization of water in the wheat kernel (Fortes *et al.*, 1981):

$L_o = 3.11\times10^6 - 2.38\times10^3 T$ $\quad L_w = R_v T^2 / H \times \partial H/\partial T$ $\quad L_v = L_w + L_o$ (J/kg)

⇒ Isotherm equation (modified Henderson's equation):

$H = 1 - \exp\left(-5869\, T^{-0.7750} M^{5203} T^{-1.363}\right)$ (decimal) (Fortes *et al.*, 1981)

⇒ Kernel thermal conductivity of wheat:

$k_T = 0.1170 + 0.0011319\times(100M)/(1+M)$ (W/mK) (Brooker *et al.*, 1992)

⇒ Liquid and vapor conductivities:

$k_l = a_1 \times 4.366 \times 10^{-18} H^3 \exp(-1331/T)$ (s) (Fortes *et al.*, 1981)

$k_v = a_2 \times 6.982 \times 10^{-9}(T - 273.16)^{0.41}\left(H^{0.1715} - H^{1.1715}\right)$ (m^2/s) (Fortes *et al.*, 1981)

⇒ Specific heat of moist wheat, and water in the liquid and vapor phases.

$c_b = (1.394 + 0.0409\,(100\,M)/(1+M))\times10^{+3}$ (kJ/(kgK) (Brooker *et al.*, 1992)

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$c_1 = 4218.69\ \text{J/kgK}$ $c_v = 1919.85\ \text{J/kgK}$

⇒ Dimensions of wheat kernel (Brooker *et al.*, 1992):
L_1=1.5748mm L_2=3.2760mm

Table 1 show the air and material conditions used in this work.

Table 1 - Air and wheat experimental conditions used in this work

Air			Wheat					t
T (^oC)	H (%)	v (m/s)	M_o (d.b.)	M_{final} (d.b.)	M_e (d.b.)	θ_o (^oC)	θ_e (^oC)	(min)
87.8	5.6	1.71	0.2110	0.127	0.0165	26.0	87.8	1020

The liquid and vapor conductivities (parameters a_1 and a_2 estimated using the least square error technique, as follows:

$$ERMQ = \sum_{i=1}^{n}\left(M_{i,Num} - M_{i,Exp}\right)^2 \qquad \overline{S}^2 = \frac{ERMQ}{(n - \hat{n})} \qquad (9a\text{-}b)$$

where ERMQ is the least square error, $\overline{S}^2$ is the variance, n is the number of experimental points and $\hat{n}$ is the parameters number fitted (Figliola and Beasley, 1995). The starting point was the mathematical expression reported to Fortes et al. (1981), to k_l and k_v applied to wheat assuming like sphere. These equations were corrected to prolate spheroid multiplying this equation by a constant parameter to be obtained.

4. Results and discussions

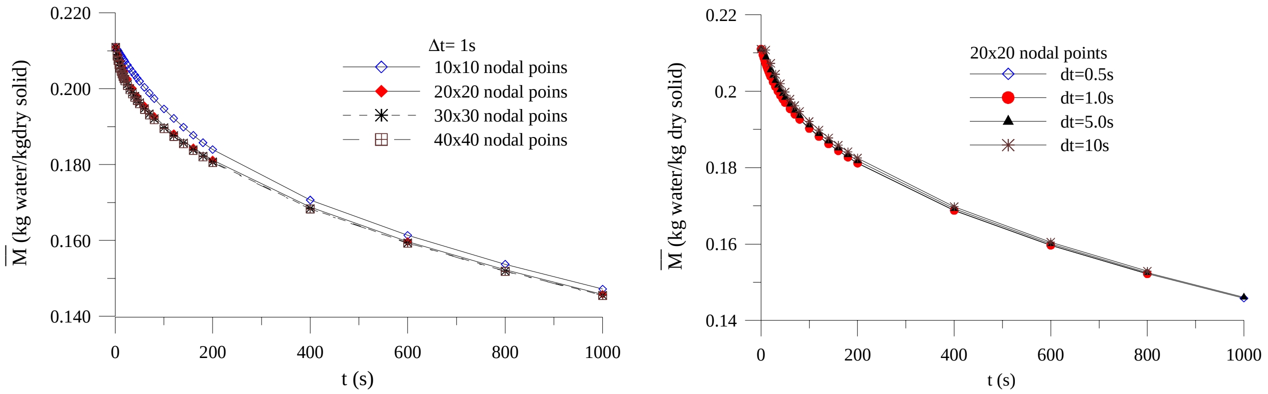
A computational code utilizing the software Mathematica® was written to solve the set of equations for the moisture content and temperature profile and to determine the average moisture content and temperature.

4.1 Grid and time step refinement

The application of the finite-volume numerical method is seriously affected by the Δt values and the number of grid points utilized in the numerical calculations. In order to verify grid size and time step independence, results were obtained with four grid sizes and time steps.The effect of mesh size on the behavior of the numerical solution for a prolate spheroid was evaluated by changing the grid size from 10x10, 20x20, 30x30 and 40x40 nodal points with Δt=1s and L_2/L_1 fixed. Except for the initial period (for the 10x10 point grid), all the grids present satisfactory results. To reach the steady state using the 40x40 point grid, the longest computational time was required. For this reason, this mesh was neglected. Figure 2 also contains the deviations between the results of the average concentration for the three grades tested and different intervals and values of the time, maintaining L_2/L_1 constant. The analysis of the results shows that the 20 x 20 point grid and the time step Δt=1s present satisfactory results. Based on these parameters, the calculation was done utilizing a uniform grid size of 20 x 20 points and a time interval of Δt=1s. The best values for spatial step and time step were obtained by successive attempts and iterations at each time. Obviously, if greater accuracy is required, other study must be conducted.

According to Lima and Nebra (2000), for prolate spheroids, the shape of the mesh varies with L_2/L_1. When $L_2/L_1 \rightarrow \infty$, the focal point is dislocated to the surface of the body; the inverse occurs for $L_2/L_1 \rightarrow 1$, when the focal point tends to coincide with the geometrical center of the body. On the zy plane, the control volumes are not uniformly spaced, presenting a bigger concentration near the surface of the body relative to ξ (radial coordinate), and on the y axis relative to η (angular coordinate). This characterizes an irregular grid; however, in the ξη 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 all the numerical calculations are performed. On the zy plane, the control volumes are not uniformly spaced, presenting a bigger concentration near the surface of the body relative to ξ (radial coordinate), and on the y axis relative to η (angular coordinate). This characterizes an irregular grid; however, in the ξη 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 all the numerical calculations are performed.

In the numerical stability analysis performed, only the finite-volume approach inside the solid was considered, and we do not have mechanisms to predict the influence of the boundary conditions on numerical stability. The boundary values have large influence on grid spacing only at the nodal points immediately near the surface of the body, in spite of the elliptic character of Equations 4a and 6a.



a) b)

Figure 2. Refinement study. a) Grid size and b) time step

4.2 Moisture transport and temperature of the wheat grain

How application and to validate the mathematical model, numerical results were compared with experimental data of the moisture content obtained during the wheat drying reported by Fortes et al. (1981), as illustrated in the Figures 3.

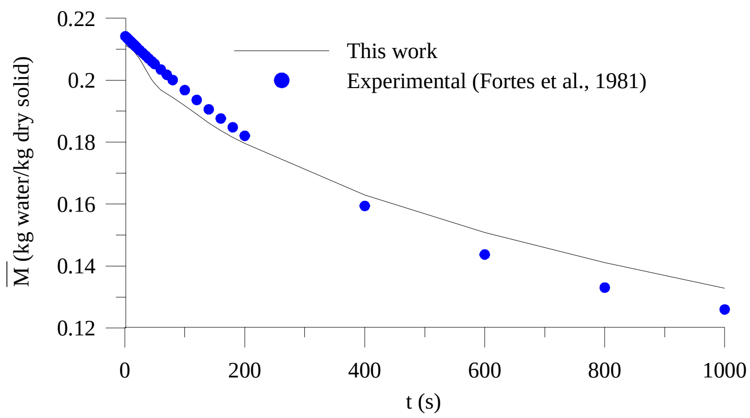


Figure 3. Comparison between predicted and experimental dimensionless

It is verified that wheat reach the equilibrium temperature i$_{in}$ ≈ 50 s, due to the boundary condition used in this work. Figure 4 show the mean temperature of the wheat during drying process. Figures 5 illustrates the behavior of the liquid and vapor flux at the surface of the solid along the drying. The numerical results showed that, vapor flux is dominant ($J_v/J_l > 10^4$), at the surface of the solid in the drying conditions used in this work. Thus, an assumption of either liquid or vapor flux, as the dominant mechanism for moisture migration in wheat is unrealistic physically.

4.3 Moisture content and temperature distributions

The moisture content distribution inside the solid is very important in order to study the evolution of mechanical stress developed in the body due to the high moisture gradients. Figures 6a-c shown the moisture content distribution inside the wheat grain exposed to the drying for 100s, 600s and 1000s, respectively. It can be seen that the highest moisture gradients happen near the surface. There is a strong drying also closed to the focal point. Then these areas are more susceptible to have troubles such as cracks and fissures, due to higher moisture gradients and shrinkage velocity. It can also be seen that a moving evaporation front occurs of the surface to center of the solid. Figures 7 a- b present the temperature distribution inside of the wheat kernel after having heated up for 10s and 20s, respectively. The highest temperature gradients happen in the proximity of the focal point, turning this area more susceptible to thermal stresses, that will contribute to the appearance of crack and fissures, besides supplying to the product the possibility to alter its color, texture and flavor, reducing this way its quality. In every drying time, may be observed that the behavior of the isothermal lines is similar from the presented by the constant moisture content lines inside of the solid. Being compared the temperature gradients with the moisture content gradients inside of the wheat (Figures 6a-c), it can be verified that these last ones are more pronounced, and the drying occurs under isothermal process for t > 50s of elapsed time.

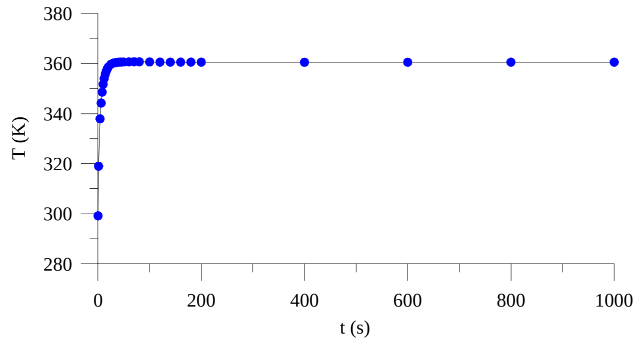
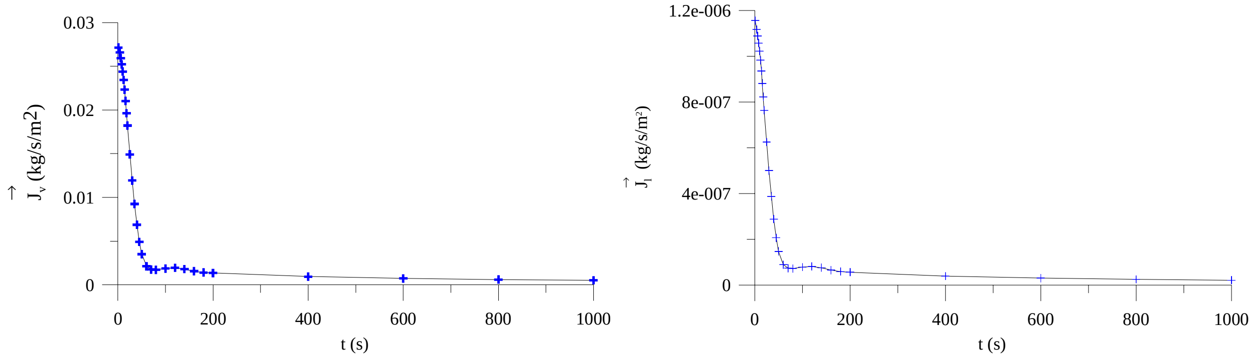
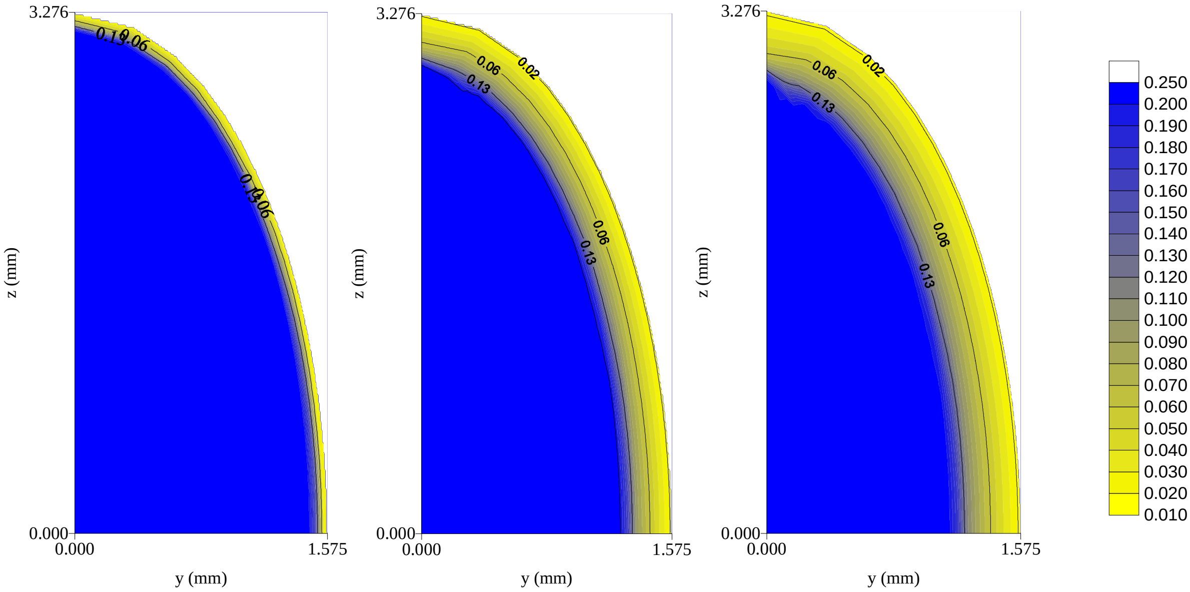


Figure 4. Predicted mean temperature of the wheat during the drying process.



a) b)

Figure 5. Predicted (a) flux liquid and (b) flux vapor at the wheat kernel surface at 87.8°C

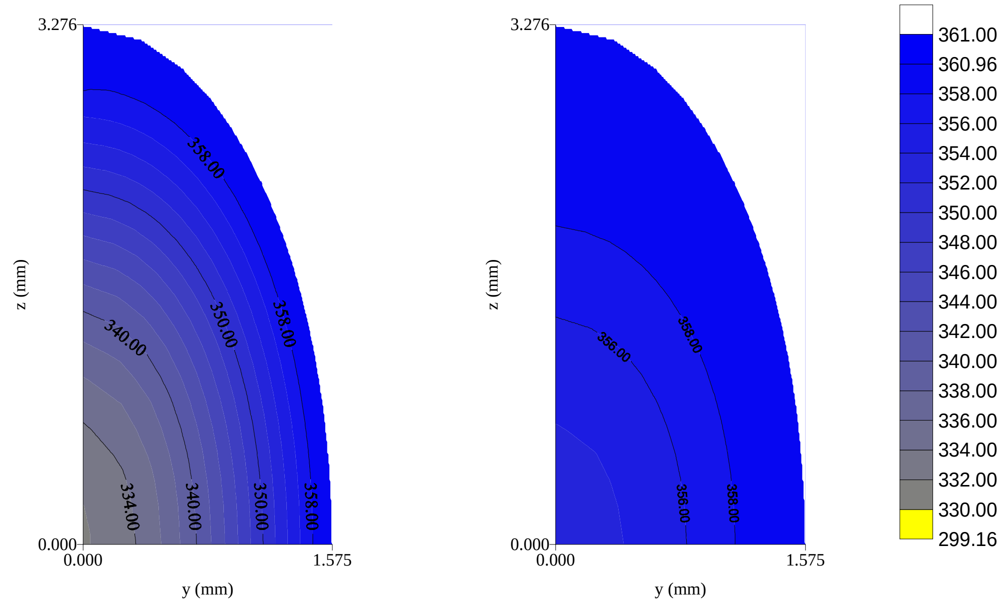


(a) t= 100s (b) t= 600s (c) t=1000s

Figure 6. Predicted moisture content distribution (dry basis) inside the wheat kernel at 87.8°C.

4.4 Transport coefficients

Table 2 presents the transport coefficients (k_l and k_v) well as the residual error (ERMQ) obtained in the simulation. The small variance indicates that the model presents good agreement with the experimental data. In general, the comparison between the transport coefficients reported in the literature is difficult due to the different models and calculation methods used, and also due to unlike composition and physical and chemical structure of the material.For a comparison, the values of the liquid and vapor conductivities of wheat-water system obtained in this work may be compared with those reported by Fortes *et al.* (1981), in the drying conditions presented in Table 1. Fortes *et al.* (1981), considers wheat like sphere. How Fortes and Okos's model was used in these works, the difference between the values may be attributed mainly to the factors: geometry assumptions; boundary conditions and convective terms in the formulation. On the other hand, during the drying phenomenon, the grain shrinks. This modifies the shape of the body, it decreases the area of heat and transfer and it increases the superficial roughness of the material. This last characteristic provides an increase of the turbulence level in the boundary layer, favoring this way the change of energy between the air and the material. Therefore of exposed, due to the good agreement obtained by comparison, we can say that the model is satisfactory to predict the liquid and vapor diffusion phenomenon in prolate spheroidal solid.



(a) t= 10s (b) t=20s

Figure 7. Predicted temperature distribution (K) inside the wheat kernel at 87.8ºC.

Table 2 – Liquid and vapor conductivities and residual error obtained in the agreement.

	This work	Fortes et al. (1981)	ERMQ $(x10^{+4})$	k_l (This work)/k_l (Fortes et al., 1981)
k_l	$k_l = a_1 \times 4.366\times10^{-18} H^3 \exp(-1331/T)$	$k_l = 4.366\times10^{-18} H^3 \exp(-1331/T)$	5.7484	a_1=19.61
k_v	$k_v = a_2 \times 6.982\times10^{-9}(T-273.16)^{0.41}(H^{0.1715} - H^{1.1715})$	$k_v = 6.982\times10^{-9}(T-273.16)^{0.41}(H^{0.1715} - H^{1.1715})$		a_2=2.68

As a final comment, it can be said that although good fit have been obtained in this study, it is necessary to pay more attention to the quantitative study of superficial area and volume changes during the dehydration processes, especially in complexes situations, such as multi directional deformations and temperature changes happen simultaneously.

5. Conclusions

Fundamentals equations for the heat and moisture diffusion in prolate spheroidal bodies, considering liquid and vapor moisture migration, were developed. The finite-volume method was used to solve the equations applied to predicted wheat drying process. From the analysis of the results obtained, the conclusions may be summarized as follows: a) the model and the technical used has great potential and it is accurate and efficient to simulate many practical problems of diffusion such as heating, cooling, wetting and drying in prolate spheroidal solids, including spheres as limit case; b) highest moisture and temperature gradients in the wheat are found near the surface and around the focal point; c) To low moisture content of wheat, the dominant migration mechanics is the vapor flux, at the surface of the solid. This work show, the facilities of the methodology to be applied for other bodies, change the aspect ratio only, compared with the solution of the diffusion problem in sphere and cylinder. In these cases, it is necessary different diffusion equations applied to the each geometry specified.

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6. Acknowledgements

The authors would like to express their thanks to CAPES (Coordenação de Aperfeiçoamento de Pessoal de Nível Superior, Brazil) and CNPq (Conselho Nacional de Desenvolvimento Científico e Tecnológico, Brazil) for supporting this work, and also grateful to the authors of the references of this paper that it helped in the improvement its quality.

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