GEOMETRY EFFECT ON WATER DIFFUSIVITY ESTIMATION IN PROINTA-ISLA VERDE AND BROOM WHEAT CULTIVARS

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***Abstract* — The effect of geometry representation of the grain kernel in the estimation of the effective diffusion coefficient of water in wheat, cv. Broom, is studied. Isothermal thin layer drying is assumed. The two-dimensional diffusive mass transport equation is solved for spherical and ellipsoidal geometries. The effective diffusion coefficient was estimated for drying air temperatures of 64, 70 and 75°C and initial grain moistures of 0.22, 0.25 and 0.28 db. Results were correlated by means of Arrhenius-type functions, varying from 2.953×10^{-11} to 6.687×10^{-11} m^2/s for ellipsoidal geometry and from 3.336×10^{-11} to 7.772×10^{-11} m^2/s for spheres. An average ratio of diffusion coefficients for ellipsoid to those for spheres was calculated to be about 0.85, very close to the value of 0.86 obtained in a previous work for the "PROINTA-Isla Verde" wheat cultivar. This ratio can be considered to be equal to the wheat sphericity squared.**

***Keywords* — Wheat, Thin layer drying, Diffusivity estimation.**

I. INTRODUCTION

The estimation of effective transport parameters in grains is usually based on experimental data of the mean moisture content evolution (oven moisture determinations) and not on local intragranular values or measured gradients**.** Diffusive kinetic models are used to interpret the phenomenon of drying, and thus the estimated values will be affected by the model hypothesis: geometry, boundary conditions, constant or variable physical and transport properties, isothermal or non isothermal drying.

Recently, Gastón *et al*. (2002) reported a study of the effect of geometry representation of the grain kernel in the estimation of the effective diffusion coefficient of water in wheat, during desorption. The results obtained for wheat cv. "PROINTA-Isla Verde", by considering the grain as sphere and axisymmetric ellipsoid showed that differences between estimated parameters may be related with grain sphericity. Some authors (Aguerre *et al*., 1987; Kang and Delwiche, 2000) had proposed that diffusivities in both geometries are related to sphericity squared, but it is understood here that evidence was not yet provided to support that assumption. To verify this observation and the trend of Gastón *et al*. (2002), the present work extends the study by including measured data on a different variety, the spring wheat cv. *Broom*. Data was collected in a different thin layer drying rig, fitted with tray weighing "in situ" and infra-red pyrometry (Bruce, 1985, 1992). Isothermal thin layer drying of wheat is assumed, for the sake of consistency with previous work. Spherical and axisymmetric ellipsoidal geometry are assigned to the grain body and the two-dimensional diffusive mass transport equation is solved applying the Finite Element Method (FEM). The effective diffusion coefficient is estimated by minimizing the sum of squares of the residuals between numerically predicted and experimental average grain moistures.

II. MATHEMATICAL MODEL

If an isothermal process is considered, the variation of moisture content inside the grains can be represented by:

$$\frac{\partial W}{\partial t} = D\,\nabla^2 W \qquad in \quad \Omega, \tag{1}$$

$$W(t=0) = W_0 \qquad in \quad \Omega, \tag{2}$$

$$W = W_e \quad on \quad \Gamma, \tag{3}$$

where Ω represents the complete domain of the grain body and Γ its boundary surface. The grain is assumed as homogeneous and isotropic material experiencing negligible volume changes and keeping a constant mass diffusivity during drying. The boundary condition described by Eqn. (3) implies that at the grain surface the equilibrium moisture content W_e is attained instantaneously. This strict internal control for wheat drying was found for this conditions using a Biot number analysis (Giner and Mascheroni, 2001). The Modified Henderson-Thompson equation with parameters for hard wheat is applied to calculate the value for W_e (Brooker *et al*., 1992). The isothermal drying assumption was taken based on the knowledge that the relaxation rate of the heat transfer potential (represented by the thermal diffusivity) is about 6000 as high as that for the mass transfer potential (diffusion coefficient) (Giner and Mascheroni, 2001) and for consistency with the previous work by Gastón *et al*. (2002)

The solution of the model is based on the finite element method for the discretization of the two-dimensional domain and a Crank-Nicholson finite difference scheme for the time variable (Segerlind, 1984). Assuming that the variation of density is negligible, average grain moisture content is calculated from nodal values according to Haghighi and Segerlind (1988).

III. GRAIN CHARACTERIZATION AND EXPERIMENTAL DATA

Unlike the thin layer drying equipment used for the “PROINTA-Isla Verde” cultivar (Gastón *et al*., 2001, 2002; Giner and Mascheroni, 2001, 2002) the dryer comprised a circular pan of area 0.2 m^2 suspended from an electronic balance in a downward flow of air. The air speed, temperature and humidity were closely controlled. An infrared pyrometer was used to measure the surface temperature of the sample under test. To eliminate the influence of air pressure on sample mass, air was diverted away from the sample and through a bypass 5 s before a weight measurement was made and restored immediately afterwards. An air speed of $0.64 ms^{-1}$ was used (Bruce and Sykes, 1983).

Operating conditions for thin layer wheat drying are reproduced in Table 1, where T_a, and h_{ra} are the temperature and relative humidity, while W_e is the grain equilibrium moisture content.

The pycnometric volume (V_g) of Broom grains was measured for each moisture content and used to assign spherical and ellipsoidal shapes to represent the kernel. In the first case, the equivalent spherical diameter (d_e) was calculated, corresponding to a sphere of the same pycnometric volume as the grain.

In the second case, an equivalent ellipsoid of revolution was considered so that its geometric volume equals the pycnometric volume. The ellipsoid dimensions l_1 (long axis) and l_m (short axis) were calculated by the following equations:

$$V_g = \frac{\pi}{6} l_1 l_m^2 \quad ; \quad \frac{l_1}{l_m} = 2 , \qquad (\mathbf{4})$$

Table 1. Experimental conditions of thin layer drying runs for Broom variety

	W_{01}= 0.2220 db		W_{02}= 0.2528 db		W_{03}= 0.2849 db	
T_a [C]	h_{ra} [dec.]	W_e [db]	h_{ra} [dec.]	W_e [db]	h_{ra} [dec.]	W_e [db]
64	0.0623	0.0395	0.0624	0.0394	0.0648	0.0401
70	0.0481	0.0344	0.0481	0.0344	0.0484	0.0345
75	0.0388	0.0307	0.0388	0.0307	0.0402	0.0312

The ratio of long to short axis was kept equal to 2, an average measured value reported for *Triticum aestivum “PROINTA-Isla Verde”* (Giner and Denisienia, 1996) and other wheat varieties (Kang and Delwiche, 1999), corresponding to an sphericity (f_e) of 0.92, (i.e, $f_e^2 = 0.85$). Values of d_e , l_1 and l_m so obtained were correlated with moisture and the results are shown in Table 2. It must be emphasized that these magnitudes were calculated for the initial moisture content values $(W = W_0)$ of Table 1, being kept constant during the application of the finite element resolution to each drying run. This procedure allows to reduce any effect likely to be caused by the small shrinkage - the specific surface area varies by 6% in the moisture range of wheat drying- and is consistent with the method followed by Gastón *et al*. (2002).

IV. RESULTS AND DISCUSSION

In previous works, Gastón *et al*. (2001; 2002) showed that when the mass diffusivity estimated with spherical geometry is used to predict drying curves assuming the grain as an axisymmetric ellipsoid, the predicted drying rate is higher than the experimental one.

This effect is explained by the fact that, being the volume for both geometries equal to the grain volume, the surface area for mass transfer is greater for ellipsoids than it is in the sphere.

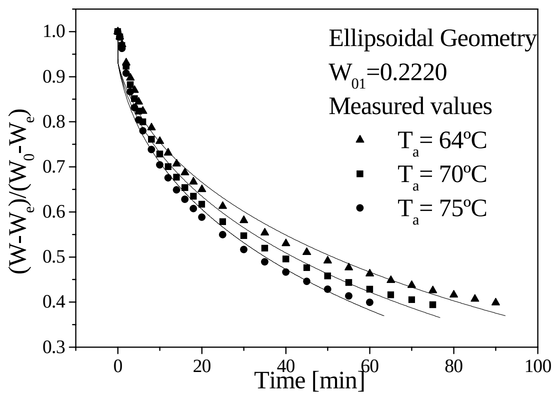
Table 2. Parameters of the linear correlation *(L = A+BW)*, of equivalent diameter *(d_e)*, long *(l_1)* and geometric average short axis *(l_m)* with moisture content for Broom variety. *(L= d_e, l_1,,l_m)*

L = A+BW		A [mm^3 or mm]	S(A)	B [mm^3or mm/db]	S(B)	r	SD
V_g		12.54	2.31	70.1	9.23	0.991	0.392
Sphere	D_e	3.11	0.011	2.98	0.042	0.999	0.002
Ellipsoid	l_1	4.93	0.02	4.76	0.06	0. 999	0.002
Ellipsoid	l_m	2.46	0.01	2.38	0.03	0. 999	0.001

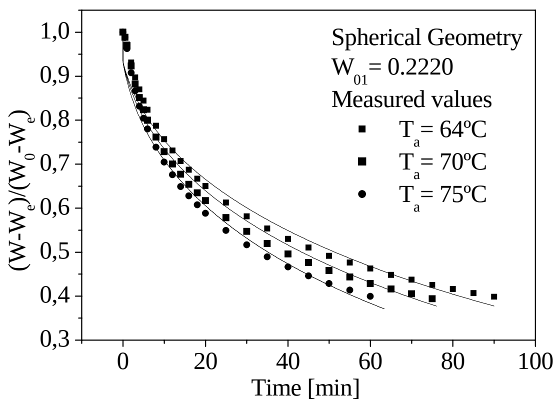
Thus, diffusion coefficients have to be obtained for each geometry from the finite element resolution of the two dimensional diffusion equation. To do so, the effect of mesh density on the average moisture content was studied and finally 196 triangular elements used to perform calculations (Gastón *et al.*, 2001). The accuracy of the finite element program was previously tested showing very good agreement between numerical and analytical solutions.

For each geometry, by minimizing the sum of squares of the residuals between numerically predicted and experimental moistures, the effective mass diffusivity was estimated as a function of the drying air temperatures for the different initial grain moisture contents listed in Table 1.

Figures 1a and 1b show the predictions obtained for some of the experiments. It can be seen that the model overpredicts the rate of moisture variation at the early stages of drying.



(a)



(b)

Fig. 1. Comparison of experimental data and numerical solution for ellipsoidal (a) and spherical (b) geometry, cv. Broom.

This effect is a consequence of the type of boundary condition imposed on the surface enhanced by the spatial discretization at the beginning of the simulation. Nevertheless, the standard deviation of the estimate of the mean moisture content varied from 0.2 to 0.9% db over the 18 experimental runs, which indicates very good predictions.

The coefficients estimated for each geometry were correlated by means of Arrhenius-type functions. Figure 2 displays the diffusion coefficients fitted with the FEM numerical scheme and the corresponding Arrhenius lines for each value of W_0, as a function of the reciprocal of the absolute temperature. It can be seen that the diffusion coefficients for the sphere are always slightly higher than they are for ellipsoid, to compensate its less extended surface compared to that of the ellipsoid of the same volume. Values obtained for the preexponential factor (D_∞) and activation energy (E_a) are listed in Table 3. The correlation coefficient r was always above 0.99 indicating accurate fitting. For these drying conditions, the effective diffusion coefficient of water in wheat varied from 2.953×10^{-11} to 6.687×10^{-11} m^2/s for ellipsoidal geometry and from 3.336×10^{-11} to 7.772×10^{-11} m^2/s in spheres.

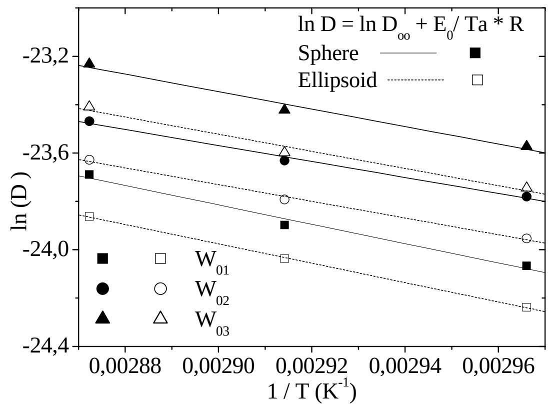


Fig. 2. Comparison of Arrhenius-type correlation of cv. Broom diffusion coefficients for sphere and ellipsoid geometry

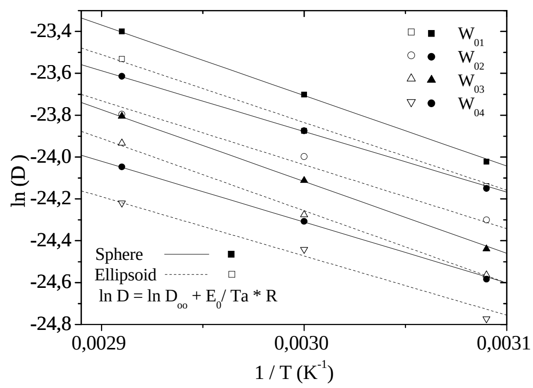


Fig. 3. Comparison of Arrhenius-type correlation of cv. Prointa Isla Verde diffusion coefficients for sphere and ellipsoid geometry.

Table 3. Parameters of the Arrhenius model $D = D_\infty \, Exp(-E_a/RT_a)$ for the thin layer drying of wheat cv. Broom (r > 0.99 in all cases)

Broom	Sphere				Ellipsoid			
W_0 [dec,db]	$D_\infty \, 10^7$ [m²/s]	$S(D_\infty)10^7$ [m²/s]	E_o [cal/mol]	$S(E_o)$ [cal/mol]	$D_\infty \, 10^7$ [m²/s]	$S(D_\infty)10^7$ [m²/s]	E_o [cal/mol]	$S(E_o)$ [cal/mol]
0.2220	49.71	71.9	7950.03	984.104	42.8299	10.70	7958.34	176.79
0.2528	8.48	7.14	6570.09	573.65	11.094	7.613	6865.27	467.35
0.2849	25.8	35.39	7179.65	934.22	17.896	25.23	7049.61	960.57

Table 4. Parameters of the Arrhenius model $D = D_\infty \, Exp(-E_a/RT_a)$ for the thin layer drying of wheat cv. “PROINTA-Isla Verde” (r > 0.99 in all cases)

Prointa	Sphere				Ellipsoid			
W_0 [dec,db]	$D_\infty \, 10^7$ [m²/s]	$S(D_\infty)10^7$ [m²/s]	E_o [cal/mol]	$S(E_o)$ [cal/mol]	$D_\infty \, 10^7$ [m²/s]	$S(D_\infty)10^7$ [m²/s]	E_o [cal/mol]	$S(E_o)$ [cal/mol]
0.1891	2.115	0.610	5902.04	191.5	1.435	0.71	5767.09	320.13
0.2133	12.88	3.047	6984.06	157.6	11.987	2.39	7029.13	129.89
0.2396	3.197	1.837	5903.87	381.4	4.395	2.09	6219.66	308.67
0.2694	16.01	6.362	6838.9	264.6	7.369	2.89	6434.05	254.84

Figure 3 and Table 4 reproduce the values previously estimated for wheat cv. “PROINTA-Isla Verde” (Gastón *et al.* 2002). Thin layer experiments were carried out for drying air temperatures of 35, 50, 60 and 70°C and initial grain moistures of 0.2694, 0.2396, 0.2133 and 0.1891 dec., db.

The Arrhenius correlation of Table 3 (cv. Broom) and Table 4 (cv. PROINTA-Isla Verde) show an apparent irregular behaviour of the pre-exponential factor D_∞, and to lesser extent, of the activation energy E_a, when analyzed for different initial moisture contents. However, Fig. 2 shows that, on the whole, D increases with W_0 for Broom, in agreement with the results obtained before for the “PROINTA Isla Verde” cultivar (Gastón *et al.*, 2001; 2002). The higher standard deviations for the preexponential factor in Broom may be caused by the fewer temperatures used, compared with the four of PROINTA-Isla Verde. The correlations obtained for Broom were used to calculate the ratio of diffusion coefficients for ellipsoid ($D_{ellipsoid}$) to those for spheres (D_{sphere}), whose average was 0.85, very close to the value of 0.86 obtained for the cv. "PROINTA-Isla Verde” in the previous work mentioned above. These ratios were plotted in Figure 4 as a function of the reciprocal of the absolute temperature for both varieties. On average, diffusion coefficient for ellipsoids resulted 14.5% below those for spheres. These differences represent a measure of the effect of geometry on the estimation of the effective diffusion coefficient for wheat. This results would confirm that $D_{ellipsoid}/D_{sphere} \sim f_e^2$ as it was proposed in previous works.

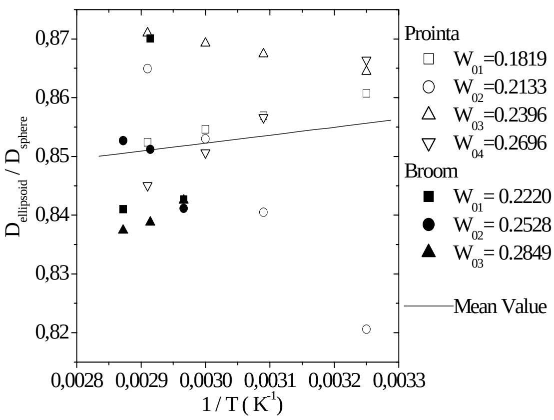


Fig. 4. Ratio of effective diffusion coefficients obtained with ellipsoidal geometry to that found with spherical shape.

V. CONCLUSIONS

Values of the effective diffusion coefficients estimated by fitting numerical predictions to experimental values of the mean moisture content depend on the geometry chosen to represent the grain. The correlation of the differences in transport properties obtained from ellipsoidal or spherical geometries can be important to correct coefficients currently used in fixed bed drying models, which, for simplicity, consider the grain as a spherical particle.

For Broom variety, the effective diffusion coefficient of water in wheat varied from 2.953×10^{-11} to 6.687×10^{-11} m^2/s for ellipsoidal geometry and from 3.336×10^{-11} to 7.772×10^{-11} m^2/s in spheres. The average ratio of diffusion coefficients for ellipsoid to those for spheres was 0.85, very close to the value of 0.86 previously obtained for the cv. "PROINTA-Isla Verde".

The results of this work, based on experimental data, numerically confirmed that the ratio of diffusion coefficients for ellipsoid to those for spheres can be considered equal to sphericity squared. The estimated average value for sphericity in "PROINTA-Isla Verde" and Broom wheats was $f_e = (0.92 \pm 0.04)$.

NOTATION

D	mass diffusivity (m^2/s)
d_e	equivalent spherical diameter (m)
D_∞	preexponential factor for mass diffusivity Arrhenius model (m^2/s)
E_a	activation energy for mass diffusivity Arrhenius model (cal/mol)
f_e	grain sphericity
h_{ra}	air relative humidity
l_1	ellipsoid long axis (m)
l_m	ellipsoid short axis (m)
r	correlation coefficient
R	universal gas constant
S	parameter standard error
SD	standard deviation of the fit
t	time (s)
T_a	ambient temperature (C)
V_g	pycnometric volume (m^3)
W	moisture content (dry base, kg / kg dry)
W_0	initial moisture content (dry base, kg / kg dry)
W_e	equilibrium moisture content (dry base, kg / kg dry)
Γ	grain boundary surface
Ω	complete domain of the grain body

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