MOISTURE DIFFUSION MODELING OF WHEAT KERNELS DURING SOAKING

S. Kang, S. R. Delwiche

ABSTRACT. *A finite element moisture diffusion model was refined for the purpose of examining the distribution of moisture within single mature kernels of wheat. Among the gross kernel components (endosperm, pericarp, and germ), moisture diffusion coefficients of the endosperm and pericarp were determined from soaking experiments and optimized with a finite element model. Nine commercial varieties of wheat, representing six U.S. market classes or subclasses, were examined. Through separate soaking experiments of pearled wheat, which represented the endosperm alone, and intact wheat, which represented the pericarp by mathematical subtraction (neglecting the contribution from the germ), the ranges in diffusion coefficients across the nine varieties were as follows:* $0.46 \times 10^{-10} - 1.4 \times 10^{-10}$ m^2/s *for endosperm,* $0.042 \times 10^{-10} - 0.42 \times 10^{-10}$ m^2/s *for pericarp. During finite element modeling, spherical and ellipsoidal geometries were assumed for pearled and intact kernels, respectively. With the kernel moisture ratio defined as the overall moisture content normalized with respect to the level of moisture at equilibrium, the soft varieties ('Rely', 'Penawawa', and 'Vanna') demonstrated a higher ratio than the hard variety 'TAM107'. Agreement between modeled and measured values for overall moisture content was very good, as seen by the ranges in the standard deviation of differences which were 0.014-0.041 and 0.008-0.029% d.b. for pearled and intact kernels, respectively. Knowledge gained from this study will be useful in understanding how the tempering process affects the milling of hard and soft wheats.*
Keywords. *Wheat, Kernel, Finite element, Diffusion coefficient, Moisture distribution.*

Tempering is a wheat moistening process that enhances milling efficiency. Control of this process may be improved with better knowledge of the distribution and movement of moisture within the wheat kernel. In tempering, temperature, variety, kernel size, and time of exposure affect the rate at which moisture enters the wheat. Among these factors, temperature has been shown to have the greatest effect, with an increase in temperature resulting in an increase in the rate of moisture absorption (Swanson and Pence, 1930; Fraser and Haley, 1932). Tempering results in a toughening of the pericarp, such that fewer small pericarp particles are formed during break. However, as tempering moisture within the kernel increases, the flour extraction rate decreases, thus necessitating that a balance be achieved between the tempering procedure and the acceptable level of bran in the flour. (Butcher and Stenvert, 1973; Hook et al., 1982a,b,c). Glenn et al. (1991) measured the compressive strength, modulus of elasticity, and energy and strain to compressive failure of wheat endosperm cylinders (1-mm diameter × 3-mm length). As moisture content increased, the compressive strength, modulus of elasticity, and energy decreased, while strain increased.

After Babbitt (1949) assumed a wheat kernel as a homogeneous sphere in order to calculate water vapor diffusion coefficient and moisture content, other researchers followed his method to obtain diffusion coefficient values for intact kernels subjected to soaking (Becker and Sallans, 1956; Jaros et al., 1992). Some drying experiments (Becker and Sallans, 1955; Chang et al., 1994) were conducted to obtain diffusion coefficients of an intact wheat kernel using the same geometrical assumption. A general solution of the diffusion equation for a wheat kernel of arbitrary shape was developed by Becker (1959). The solution in the neighborhood of time zero has been used to determine the diffusion coefficient of an intact wheat kernel (Becker, 1960; Fan et al., 1961; Glenn and Johnston, 1994). Recently, Igathinathane and Chattopadhyay (1997) assumed a spherical shape for a kernel and used the finite difference method to determine the diffusion coefficients of the endosperm and pericarp. Their model was used in conjunction with moisture gain measurements of immersed whole and pearled wheat. Because the actual shape of wheat kernels is not spherical, it is suspected that, as Muthukumarappan and Gunasekaran (1990) determined for corn kernels (with trials involving an infinite cylinder, an infinite slab, and a sphere), geometrical shape has a significant effect on numerically derived diffusion coefficient values for wheat endosperm and pericarp. An alternate method to determine the moisture diffusion coefficient of wheat endosperm is nuclear magnetic resonance (NMR) (Callaghan et al., 1979; Jenner et al., 1988; Eccles et al., 1988; Jenner and Jones, 1990). Although the NMR method can provide detailed

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information on moisture movement within endosperm slices, lengthy experimentation times are required, and the destructive aspect of slicing does not permit the observation of moisture on an *in-situ* basis except in the case of using very expensive three dimensional NMR imaging instrumentation.

Hinton (1955) measured the rates of water movement through different regions of the wheat kernel and found that the rates within the pericarp were lower than other regions including the endosperm, thus demonstrating that the different components of a wheat kernel have different diffusivities. He reported that the testa of the pericarp was the limiting barrier for moisture absorption. Glenn and Johnston (1994) confirmed that studies of moisture diffusivity in intact wheat could provide little information on the actual diffusivity of endosperm. Therefore, because a wheat kernel is heterogeneous (i.e., endosperm, pericarp, and germ) and is not spherical in shape, analytical solution of diffusion coefficients of these components simultaneously is not possible. Hence, the finite element method along with computer technology advances is a practical approach for geometrically complex and non-uniform material properties of wheat kernels.

In this study, a finite element model was applied to determine the diffusion coefficients of wheat endosperm and pericarp during isothermal moisture soaking. After determining the diffusion coefficients, moisture content distribution was predicted. The overall objective of this research was to understand the dynamics of moisture uptake within the wheat kernel during tempering. The specific objectives were to (1) determine values for diffusion coefficients of the endosperm and pericarp of wheat from various classes during moisture tempering, and (2) develop a finite element diffusion model to predict moisture migration and distribution within the wheat kernel.

Theoretical Considerations

Diffusion Equation and Boundary Condition

When diffusion in a wheat kernel takes place at constant temperature and pressure, the moisture diffusion follows Fick's second law. The governing equation for axisymmetric diffusion equation is given as follows (Crank, 1975):

$$D\left(\partial^2 m/\partial r^2 + \partial m/(r\partial r) + \partial^2 m/\partial z^2\right) = \partial m/\partial t \qquad (1)$$

where

D = diffusion coefficient (m^2/s)

m = moisture content (%, d.b.)

r = radial coordinate (m)

z = axial coordinate (m)

t = time variable (s)

The following assumptions are made for using equation 1:

1. The diffusion coefficient of a kernel is not a function of moisture concentration.
2. The kernel is considered isothermal and heat transfer is neglected.
3. The endosperm and pericarp of grain material are homogeneous and isotropic.
4. The volume change of the kernel is negligible during tempering process.

The boundary condition is that the kernel surface maintains an equilibrium moisture content, m_{eq}. The initial condition is that the moisture content of the entire kernel is uniform, m_{in}.

Finite Element Solution. Using a finite element approach similar to that used by other researchers of cereals and oilseeds (Irudayaraj et al., 1992; Lu and Siebenmorgen, 1992; Muthukumarappan and Gunasekaran, 1994, 1996), Galerkin's weighted residual method was used to transform the governing equation into element equations. By applying the known boundary conditions and a backward difference time scheme, the final system form of diffusion model was as follows:

$$([C] + \Delta t\,[K])\,(m)_{t+\Delta t} = [C](m)_t + \Delta t\,(F)_{t+\Delta t} \qquad (2)$$

where [C] is a global capacitance matrix, [K] is a global stiffness matrix, and (F) is a global force vector. Assuming constant density for a kernel, the mass average method (Haghighi and Segerlind, 1988) was used to determine the overall moisture content of the kernel.

Analytical Solution for Simplified Geometry. If the wheat kernel is considered a sphere, the spatial component of the diffusion equation becomes one-dimensional. For constant D and spherical geometry, the diffusion equation can be written as:

$$D\left(\partial^2 m/\partial r^2 + 2\partial m/(r\partial r)\right) = \partial m/\partial t \qquad (3)$$

Analytical solutions of equation 3 for the overall moisture content of a sphere can be obtained directly (Crank, 1975):

$$MR = \frac{\overline{m}_t - m_{in}}{m_{eq} - m_{in}} =$$

$$1 - \left(\frac{6}{\pi^2}\right)\sum_{n=1}^{\infty}\left(\frac{1}{n^2}\right)\exp\left[-Dn^2\pi^2\frac{t}{r_0^2}\right] \qquad (4)$$

where

MR = moisture ratio (dimensionless quantity ranging from 0 to 1)

$\overline{m}_t$ = average moisture content at time t (%, d.b.)

m_{eq} = equilibrium moisture content at kernel surface (%, d.b.)

m_{in} = initial moisture content of entire kernel region (%, d.b.)

r_0 = radius (m)

If $D\pi^2 t/r_0^2$ is smaller than 1.2, equation 4 with only the first term in the series is correct to within 0.05.

Procedure

Wheat

The following wheat varieties (with wheat class identified in parentheses), which originated as 1997 breeders variety trials, were obtained from USDA Wheat Quality Laboratories located in Fargo, North Dakota, Manhattan, Kansas, and Pullman, Washington: 'Grandin' [hard red spring (HRS)], 'Amidon' (HRS), 'Renville' (durum), 'Jagger' [hard red winter (HRW)], 'TAM107' (HRW), 'Madsen' [soft white winter (SWW)], 'Rely' (club), 'Penawawa' [soft white spring (SWS)], and 'Vanna' (SWS). These hard and soft varieties represent some of the most popular commercial releases grown throughout the Great Plains and Pacific Northwest regions of the United States. Samples were kept under refrigeration (ca. 5°C) prior to testing.

Experimental

For the soaking tests, intact kernels and pearled kernels were examined separately. In the latter group, wheat samples (20 g) were pearled with a Strong Scott pearler (Seedboro Equipment Co., Chicago, Ill.). A sieve (The W.S. Tyler Co., No. 8) was used to remove broken and small kernels. The shape of the pearled wheat was ellipsoidal and in some cases, nearly spherical. The lengths (a, b, c) along three principle axes were measured (table 1). The radius was one half the mean of these three lengths. All dimension designators of the wheat kernel are illustrated in figure 1. After pearling, samples were held in a room at 22°C and approximately 65% relative humidity (r.h.) for 72 h.

During the soaking experiment, both room and water temperatures were 22°C and room humidity was 55% r.h. Every 15 min, each sample (ca. 10 g) was taken from the bath, blotted on filter paper (Schleicher & Schuell Co., No. 588, 18.5-cm diameter) to remove surface moisture, weighed, and then returned to the bath. This procedure continued for a total of 240 min.

Initial moisture contents of pearled and intact wheat kernels (table 2) were measured by the oven method (130°C, 19 h), following ASAE standard S352.2. The size of each sample was approximately 10 g. Except for Penawawa, moisture contents of whole-wheat samples were slightly lower than the pearled ones. Equilibrium moisture contents of soaked wheat (data not shown) were determined at 4 and 48 h of immersion for pearled and intact kernels, respectively.

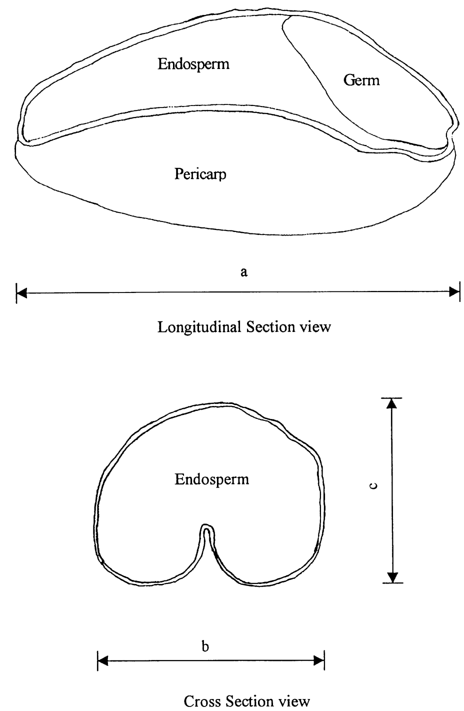

Figure 1–Structure and dimension designators of a wheat kernel.

Table 2. Initial moisture content (%, d.b.) of pearled and intact wheats

Variety	Pearled	Intact
Grandin	14.8	14.2
Amidon	13.6	13.4
Renville	14.8	14.0
Jagger	15.6	14.7
TAM107	15.7	14.9
Madsen	14.1	13.8
Rely	14.0	13.5
Penawawa	14.3	14.9
Vanna	14.5	13.8

Finite Element Modeling

Commercial finite element analysis software (MARC6.2, MARC Analysis Research Co., Palo Alto, Calif.) was used to determine the moisture diffusion coefficient and to evaluate the overall wheat kernel moisture content and distribution of moisture within the kernel. The shape of the pearled wheat kernel was assumed to be spherical while that of the intact kernel was considered to be prolate spheroidal. For pearled wheat, one quarter of a circle was used as the axisymmetric two-dimensional analysis condition.

Table 1. Kernel dimensions (mm) of pearled and intact wheats

		Pearled		Intact					
Variety	Class*	Radius†	SD‡	a†	SD‡	b†	SD‡	c†	SD‡
Grandin	HRS	1.67	0.059	5.86	0.25	3.38	0.17	3.00	0.10
Amidon	HRS	1.57	0.085	6.18	0.35	3.05	0.15	2.88	0.22
Renville	Durum	1.73	0.101	7.17	0.41	2.92	0.25	2.85	0.18
Jagger	HRW	1.68	0.048	6.17	0.52	3.22	0.16	2.91	0.17
TAM107	HRW	1.67	0.061	6.41	0.29	3.41	0.13	2.89	0.12
Madsen	SWW	1.63	0.109	6.67	0.28	3.60	0.52	3.00	0.18
Rely	Club	1.47	0.103	6.05	0.33	3.03	0.23	2.54	0.15
Penawawa	SWS	1.47	0.094	6.24	0.26	3.30	0.12	2.95	0.18
Vanna	SWS	1.64	0.063	6.47	0.28	3.20	0.13	2.74	0.14

* Hard red spring (HRS), hard red winter (HRW), soft white winter (SWW), soft white spring (SWS).
† Mean of 30 measurements (a: the longest length dimension, b: width, c: height , as defined in fig. 1).
‡ Standard deviation of dimension.

The grid for pearled wheat consisted of 160 nodes and 98 triangular elements (fig. 2). One subroutine was attached to the main MARC program to calculate the moisture diffusion coefficient. After numerous preliminary runs involving different time steps, a 15-min step was selected as adequate, based on an error analysis function in the MARC program. In the diffusion coefficient routine, across all 15-min marks, the sum of squared deviations between the overall moisture contents from the measured data and those from the finite element model with an assumed endosperm diffusion coefficient value was calculated. Based on the objective of minimizing the sum of squared deviations, the diffusion coefficient was determined using the Golden Section search method (Jacoby et al., 1972), which is an optimization algorithm. After determining the value of the endosperm diffusion coefficient for each sample, the main program calculated

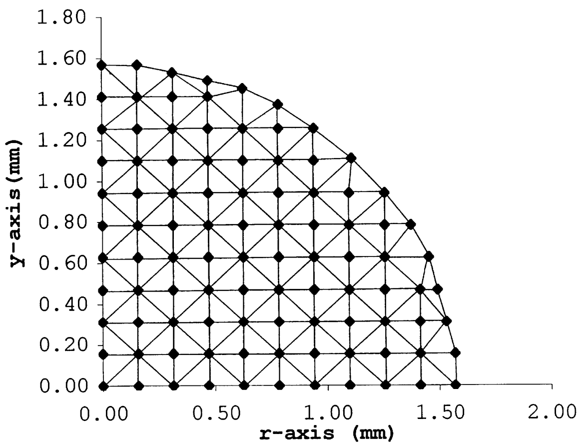

Figure 2–Finite element grid for a pearled wheat kernel.

the local moisture content at each node in a pearled wheat kernel using one-second time steps.

For the intact kernel, one-quarter of an ellipse was used in a time-dependent axisymmetric two-dimensional analysis (fig. 3). The dimensions and grid for the whole kernel are shown in table 3, where "d" is half of the longest length dimension and "e" is half of the mean value of "b" and "c" from figure 1. For all samples, the thickness of pericarp was assigned to be 0.125 mm, based on actual measurement of one variety (Bennett). For the endosperm region, the diffusion coefficient determined from the pearled wheat experiment was used. By use of the same optimization procedure as used for pearled wheat, the remaining unknown, the pericarp diffusion coefficient, was determined. The grid for intact wheat consisted of between 427 and 540 nodes associated with 271 to 307 triangular elements. The variation in numbers of nodes and elements was because of variety-to-variety size variations, as an attempt was made to make element sizes equivalent across varieties.

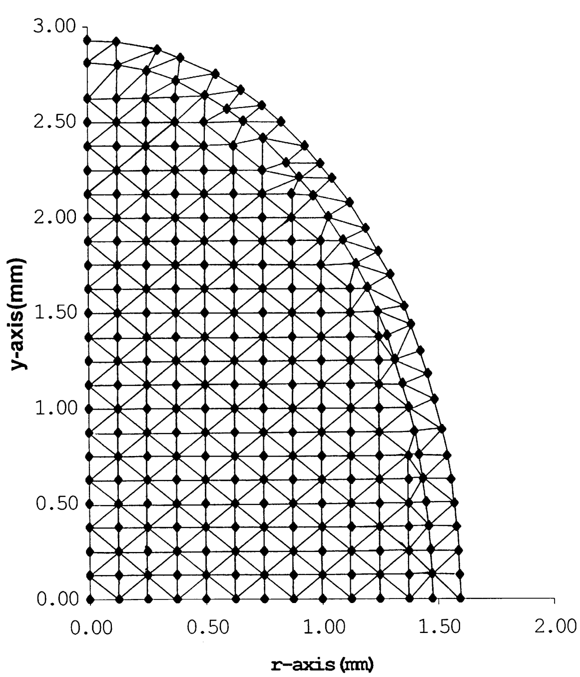

Figure 3–Finite element grid for a single intact wheat kernel.

Table 3. Dimensions and the number of nodes and elements used in the finite element procedure

Variety	d*	S.D.†	e*	S.D.†	Nodes	Elements
Grandin	2.93	0.25	1.60	0.11	477	271
Amidon	3.09	0.35	1.48	0.17	480	274
Renville	3.58	0.41	1.44	0.20	540	307
Jagger	3.09	0.52	1.53	0.13	474	270
TAM107	3.20	0.29	1.58	0.11	513	291
Madsen	3.34	0.28	1.65	0.29	552	312
Rely	3.03	0.33	1.39	0.14	427	245
Penawawa	3.12	0.26	1.56	0.12	500	284
Vanna	3.24	0.28	1.49	0.12	484	276

* Mean of 30 measurements. d is half of the longest length dimension and e is half of the mean values of b and c from figure 1.
† Standard deviation of corresponding dimension.

Upon determining values for the diffusion coefficients of the pericarp, the local moisture content at each node in the intact wheat kernel was calculated at one-second time steps. Every 15 min, the overall moisture content of the intact kernel was determined.

Results and Discussion

Moisture Ratio

Approximately 150 min after the beginning of the soaking experiment, the moisture content of pearled wheat was nearly at equilibrium status. Among the pearled wheat samples, the initial moisture content of the hard red winter varieties (Jagger and TAM107) was higher than that of other wheat classes. The moisture contents of the other pearled wheat varieties were similar (fig. 4). During the soaking experiment of intact wheat samples, the moisture ratios for TAM107 were lowest, while the soft varieties, Rely, Penawawa, and Vanna, showed higher moisture ratios than other varieties (fig. 5). The moisture absorption rates of the pearled kernels were greater than the corresponding rates of the intact kernels. The endosperm of TAM107 showed a higher moisture absorption rate than that of other varieties, while the intact TAM107 kernels showed the lowest moisture absorption rate. It appears that the pericarp of TAM107 acted as a strong moisture barrier.

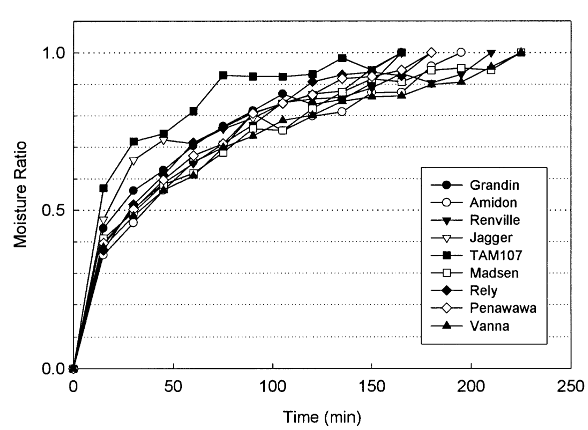

Figure 4–Moisture ratios of pearled kernels of various wheat varieties subjected to soaking.

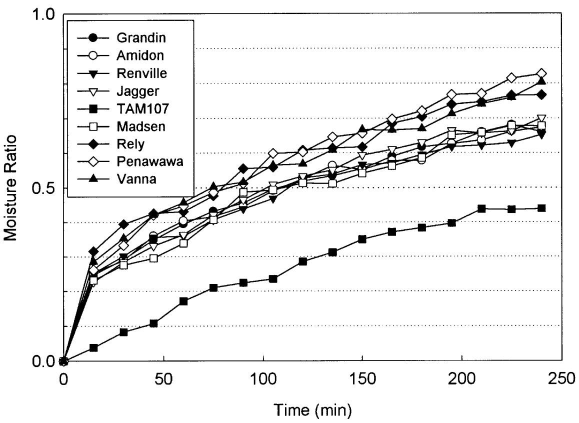

Figure 5–Moisture ratios of intact kernels of various wheat varieties subjected to soaking.

Diffusion Coefficients

Hard red winter wheat showed a higher endosperm diffusion coefficient than other classes, with soft white spring showing the lowest. Across all varieties, diffusion coefficient values of the endosperm were within the range of 0.46×10^{-10} to 1.4×10^{-10} m^2/s (table 4). Compared with other research, these values are lower than those obtained by NMR (Callaghan et al., 1979; Jenner et al., 1988; Eccles et al., 1988; Jenner and Jones, 1990) and by a recent soaking experiment (Igathinathane and Chattopadhyay, 1997) (table 5). A probable reason for the lower values is that a lower temperature (22ºC) was used in the present study, compared with temperatures of 28ºC for NMR and 30ºC for soaking. Also, compared to the NMR studies, in which the self-diffusion coefficient along the grain axis of an immature wheat kernel during the grain filling stage was measured, the current study deals only with fully mature kernels and treats the endosperm as isotropic. Thus, it is plausible that transport of water occurs more readily during the kernel's development than at full maturity. Conversely, some researchers (Becker and Sallans, 1955; Jaros et al., 1992; Becker, 1959, 1960; Fan et al., 1961) reported on diffusion coefficient values that were smaller than the values of the present study (table 5). In these cases, various forms of an analytical solution (similar to eq. 4) for a homogeneous medium, with soaking data, were applied to intact kernels.

Table 4. Diffusion coefficients [D ($m^2/s \times 10^{10}$)] of wheat endosperm and pericarp, and standard deviation (S.D.) of differences between measured and modeled moisture contents (%, d.b.) for pearled and intact wheat

		Endosperm		Pericarp*	
Variety	Class	D	S.D.	D	S.D.
Grandin	HRS	0.80	0.0210	0.13	0.0289
Amidon	HRS	0.55	0.0247	0.16	0.0276
Renville	Durum	0.73	0.0139	0.13	0.0277
Jagger	HRW	0.91	0.0301	0.13	0.0198
TAM107	HRW	1.4	0.0192	0.042	0.0077
Madsen	SWW	0.60	0.0226	0.19	0.0186
Rely	Club	0.46	0.0408	0.32	0.0197
Penawawa	SWS	0.55	0.0151	0.42	0.0093
Vanna	SWS	0.57	0.0192	0.29	0.0173

* The diffusion coefficient, D, refers to that for the pericarp alone; whereas, the standard deviation of differences, S.D., refers to the intact kernel.

Table 5. Other diffusion coefficient values from the literature

Source	Variety	Temperature (°C)	RH (%)	Diffusion Coefficient (m^2/s (10^{10}))
Becker and Sallans (1955)	Thatcher	20.8-79.5	-	0.069-7.2
Becker (1960)	Thatcher	25	-	0.018-0.031
Fan et al. (1961)	Ponca	26.7-98.3	-	0.027-2.456
	Vernum	30.-86.	-	0.022-0.752
	Seneca	26.7-98.3	-	0.031-1.409
	Brevor	30.0-86. 0	-	0.027-0.891
Callaghan et al. (1979)	Aotea (endosperm)	22	88	1.8
			99	12
Jenner et al. (1988)	Otane	-	-	8.3
Eccles et al. (1988)	Otane: Endosperm, Dorsal	28 ± 1	-	5
	Otane: Endosperm, Cheek			7
	Otane: Endosperm, Ventral			7
	Otane: Vascular bundle + chalaza			10.1
	Otane: Nucellar projection			5
	Otane: Endosperm cavity			10.6
	Otane: Aleurone layer etc.			9
Jenner and Jones (1990)	Sun 9E: Detached	22 ± 2	-	6.9-8.6
	Sun 9E: Attached			13.9-16.0
Glenn and Johnston (1994)	Arizona	30	72	0.036
	Len			0.044
	Hatton			0.029
	Triumph 64			0.024
	Larned			0.028
	Logan			0.027
	Titan			0.028
	Becker			0.025
	Augusta			0.034
	Stephens			0.023
	Arizona (endosperm)			0.02 ± 0.00062
	Len (endosperm)			0.02 ± 0.00057
	Logan (endosperm)			0.035 ± 0.0046
	Titan (endosperm)			0.091 ± 0.009
Chang et al. (1994)		0-50	-	12-2900
Igathinathane and Chattopadhyay. (1997)	Endosperm	30	-	1.92
	Bran			1.78

Therefore, the low diffusion coefficient values from these studies could reflect the effect of the pericarp acting as a barrier to moisture.

The diffusion coefficient values of the pericarp were within the range of 0.042×10^{-10} to 0.42×10^{-10} m^2/s (table 4). The diffusion coefficients of endosperm were larger than those of pericarp, which is in agreement with historical research that concluded the moisture absorption rate of endosperm is faster than that of pericarp (Hinton, 1955). Hard red winter and hard red spring wheat showed a lower pericarp diffusion coefficient than other classes, and club and soft white spring had the highest values. The diffusion coefficient of TAM107 pericarp was the lowest of all other varieties.

Predicted Moisture Ratio and Moisture Migration

Moisture Ratio (MR) for pearled wheat was predicted with the determined diffusion coefficients of endosperm from the finite element method. For example, the predicted MR values for pearled Penawawa were similar to the measured and analytical solution (eq. 4 with 35 series terms) values (fig. 6). Other varieties showed similar patterns. Based on the success of achieving close agreement between the finite element model and analytical solution for MR, the finite element method was also applied to intact wheat. The MR for intact wheat was calculated, based on the determined diffusion coefficients

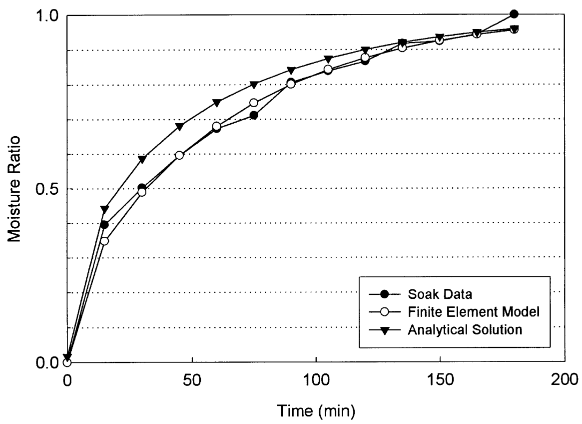

Figure 6–Comparison of moisture ratios determined by soaking, finite element analysis, and an analytical solution of the diffusion equation for pearled kernels of the variety 'Penawawa'.

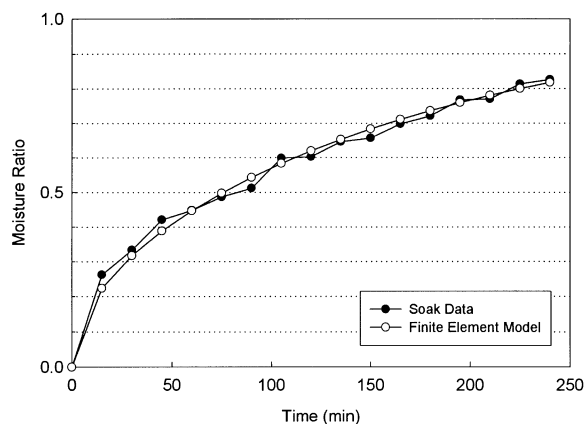

Figure 7–Comparison of moisture ratios determined by soaking and finite element analysis for intact kernels of the variety 'Penawawa'.

of endosperm and pericarp. The finite element model predicted the moisture ratio of intact wheat very well with few exceptions, as noted below (fig. 7). The level of agreement, expressed as the standard deviation of differences between predicted (eq. 4, solved for $\overline{m}_t$) and actual measurements at the 15-, 30-, . . . , 240-min readings of dry basis moisture content are contained in table 4. With values ranging from 0.014 to 0.041% d.b. for pearled kernels and 0.008 to 0.029% d.b. for intact kernels, these levels of closeness suggest that the diffusion coefficient values are reasonably accurate. At the start of the experiment, the moisture content by calculation was lower than that by direct measurement, presumably because this represented the condition of highest moisture gradient. This phenomenon was also observed by Igathinathane and Chattopadhyay (1997), using a finite difference model.

Having obtained values for diffusion coefficients of the endosperm and pericarp, the finite element diffusion models were subsequently able to provide a second-by-second glimpse of the distribution and movement of moisture within the kernel. By way of example figures 8 and 9 show the moisture distribution at 60 min for pearled wheat and intact wheat, respectively.

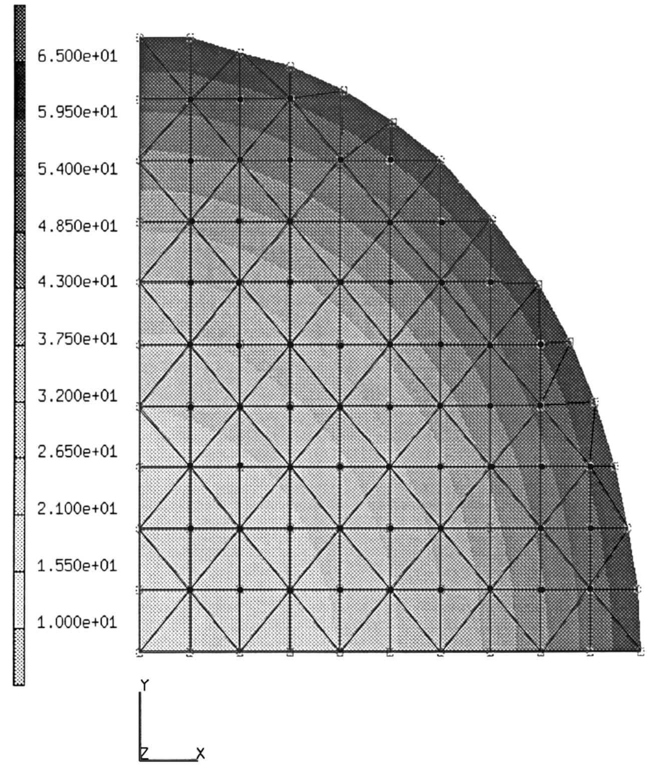

Figure 8–Typical distribution of moisture in a pearled wheat kernel, as determined by finite element analysis.

SUMMARY AND CONCLUSIONS

Moisture diffusion coefficients for wheat endosperm and pericarp were determined from both absorption experimental data and a finite element diffusion model. The moisture ratios of the soft wheats, Rely, Penawawa, and Vanna, were higher than those of other varieties. The moisture absorption pattern for TAM107 was different than that for the other varieties. The moisture absorption rate of pearled wheat (endosperm) was faster than that of intact wheat. Use of mathematical models is of great potential benefit to the wheat processing industry because the models provide information on the dynamics of moisture absorption without the need for actual measurement, thus giving the miller a method for tailoring tempering regimes to the unique characteristics of individual wheat lots. Ultimately, a better understanding of the tempering procedure through the current and future studies will lead to a clearer understanding of the relationships between wheat hardness, moisture, and milling performance

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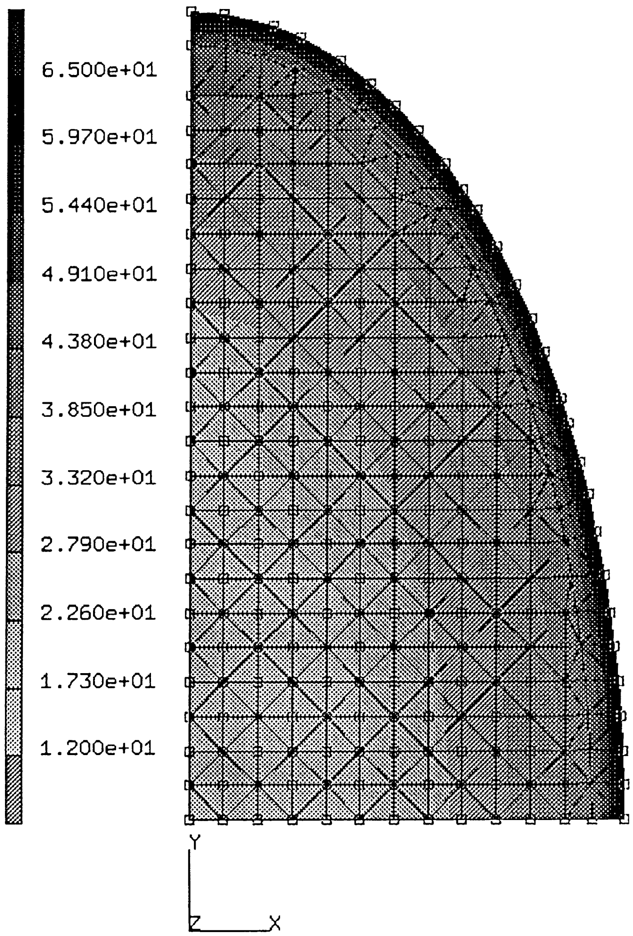

Figure 9–Typical distribution of moisture in an intact wheat kernel, as determined by finite element analysis.

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