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INVERSE DETERMINATION OF DIFFUSION COEFFICIENT FOR MOISTURE DIFFUSION IN WOOD

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ABSTRACT

This paper presents the inverse determination of the diffusion coefficient in the one-dimensional non-steady state diffusion equation using a second-order finite difference procedure. Test data of moisture desorption in northern red oak (*Quercus rubra*) were used in the numerical analysis. Results indicate that the diffusion coefficient is a function of time, position, moisture content, and moisture gradient, which is at variance with assumptions in the literature that the diffusion coefficient is either a constant or a function of moisture content only. However, experimental data in the literature that relate diffusion of certain diffusing substances in porous materials bear resemblance to our results. Consequently, the functional form of the diffusion coefficient for moisture diffusion in wood may need to be further examined.

INTRODUCTION

This paper presents the inverse determination of the diffusion coefficient in the one-dimensional non-steady state diffusion equation based on desorption test data of moisture variations in northern red oak (*Quercus rubra*) specimens (Simpson 1993). To reduce the effects of data scatter, the test data were simulated by mathematical modeling. The simulated data represent the test data very closely, except for data close to the boundary or data taken at large times, where there are some inconsistencies as a result of experimental difficulties. The simulated data with properly prescribed values at the boundary or at large times were analyzed using a second-order finite difference technique. Results show that the diffusion coefficient depends on time, position, moisture content, and moisture gradient, which is a possible situation according to Crank (1975).

In the literature on moisture diffusion in wood, some authors have assumed that the diffusion coefficient depends strongly on moisture content (e.g., Hougen et al. 1940, Meroney 1969, Simpson 1993, Skaar 1954, Van Arsdel 1947), while others have taken the diffusion coefficient as constant (e.g., Avramidis and Siau 1987, Choong and Skaar 1972, Droin et al. 1988, Mounji et a1. 1991, Soderstrom and Salin 1993). No one has ever attempted to use the inverse method to determine the diffusion coefficient. In using the inverse method, the governing partial differential equation is converted into a system of linear equations based on test data. In the system of linear equations, the unknowns are the values of the diffusion coefficient corresponding to different times and positions, which can be easily obtained. The advantage of this approach is that no prior information or assumption is required on the functional form of the diffusion coefficient.

The inverse method has been used with success to determine the thermal conductivity in heat conduction problems (Chen et al. 1996, Yeung and Lam 1996). Since the governing equations for heat conduction and moisture diffusion are the same, it is only natural to use the same procedure to investigate the diffusion coefficient in a moisture sorption or desorption process of wood. The only condition for such an application is that moisture variations with time and position in wood be known over the entire domain of interest, which, for northern red oak, are available to us in the work of Simpson (1993).

The inverse solutions are known to be very sensitive to changes in input data resulting from measurement and modeling errors. Hence, they may not be unique. Mathematically, the inverse problems belong to the class of "ill-posed problems;" that is, their solution does not satisfy the general requirements of existence, uniqueness, and stability under small changes to the input data (Özisik 1993). In the present study, the moisture desorption data of northern red oak were carefully analyzed, and we expect that the solutions should at least describe the general features of the diffusion coefficient.

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NOMENCLATURE

- a half of medium thickness, mm
- C concentration of diffusing substance, %
- C_e equilibrium concentration of diffusing substance, %
- C_0 initial concentration of diffusing substance, %
- D diffusion coefficient, mm^2/h
- S surface emission coefficient, mm/h
- t time, h
- X distance coordinate, mm
- α constant

Subscripts

- i time index
- j position index

ONE-DIMENSIONAL DIFFUSION EQUATION

In a one-dimensional formulation with the diffusing substance moving in the direction normal to a sheet of medium of thickness $2a$, the diffusion equation can be written as

$$\frac{\partial C}{\partial t}=\frac{\partial}{\partial X}\left(D\frac{\partial C}{\partial X}\right) \qquad (0<X<a, t>0) \tag{1}$$

where C is concentration of the diffusing substance, t is time, D is diffusion coefficient, and X is distance coordinate measured from the center of the sheet.

Let the initial condition be

$$C=C_0 \qquad (0<X<a, t=0) \tag{2}$$

where C_0 is a constant concentration in the medium, and let the boundary conditions be

$$\frac{\partial C}{\partial X}=0 \qquad (X=0, t\geq 0) \tag{3}$$

$$D\frac{\partial C}{\partial X}=S(C_e-C) \qquad (X\approx a, t>0) \tag{4}$$

where S is surface emission coefficient and C_e is equilibrium concentration corresponding to the vapor pressure in the environment remote from the surface of the sheet.

The main purpose of this study is to determine the diffusion coefficient $D(X,t)$ at any point within the domain of $0<X<a$ and $t>0$ with the assumption that $C(X,t)$ is known at discrete grid points, as described in the next section.

INVERSE DETERMINATION OF DIFFUSION COEFFICIENT

A finite difference procedure for the calculation of the diffusion coefficient at discrete grid points will first be presented. Then the computational algorithm for the determination of the diffusion coefficient values corresponding to different times and positions will be given.

Finite Difference Formulation

Let half of medium thickness, a, be discretized with mesh width ΔX in distance (thickness direction) and At in the time direction with grid points $X_j = j\cdot\Delta X$ (where j = 0,1,...,n) and $t_i = i\cdot\Delta t$ (where i = 0,1,2...). The present procedure will assume that $C(X,t)$ are known at grid points (X_j, t_i). Equation (1) can then be discretized as follows:

(a) At the surface grid point with $j = 0$ and $i > 0$:

Applying forward difference to the time derivative of Equation (1), we have

$$\left(\frac{\partial C}{\partial t}\right)_0^i=\frac{C_0^{i+1}-C_0^i}{\Delta t} \tag{5}$$

Applying the central difference to the distance derivative, we obtain

$$\left[\frac{\partial}{\partial X}\left(D\frac{\partial C}{\partial X}\right)\right]_0^i=\left(\frac{D_1^i+D_0^i}{2}\cdot\frac{C_1^i-C_0^i}{\Delta X}-D_0\alpha\frac{C_1^i-C_0^i}{\Delta X}\right)\Bigg/\left(\frac{\Delta X}{2}\right) \tag{6}$$

where we have set in Equation (4)

$$\left(D\frac{\partial C}{\partial X}\right)_0^i=D_0\alpha\frac{C_1^i-C_0^i}{\Delta X} \tag{7}$$

by introducing an appropriate constant a to compensate the use of forward difference in the equation, which involves different errors than central difference (Özisik 1993). This also permits us to avoid using the unknown surface emission coefficient S.

Equating Equations (5) and (6) gives

$$\frac{(\Delta X)^2}{\Delta t}\left(C_0^{i+1}-C_0^i\right)=D_0^i(2\alpha-1)\left(C_0^i-C_1^i\right)+D_1^i\left(C_1^i-C_0^i\right) \tag{8}$$

(b) At an internal grid point with $0<j<n$ and $i>0$:

Here we have

$$\left(\frac{\partial C}{\partial t}\right)_j^i=\frac{C_j^{i+1}-C_j^i}{\Delta t} \tag{9}$$

and

$$\left[\frac{\partial}{\partial X}\left(D\frac{\partial C}{\partial X}\right)\right]_j^i=\left(\frac{D_{j+1}^i+D_j^i}{2}\cdot\frac{C_{j+1}^i-C_j^i}{\Delta X}-\frac{D_j^i+D_{j-1}^i}{2}\cdot\frac{C_j^i-C_{j-1}^i}{\Delta X}\right)\Bigg/\Delta X \tag{10}$$

Equating Equations (9) and (10) yields

$$\frac{2(\Delta X)^2}{\Delta t}\left(C_j^{i+1}-C_j^i\right)=D_{j-1}^i\left(C_{j-1}^i-C_j^i\right)+D_j^i\left(C_{j+1}^i-2C_j^i+C_{j-1}^i\right)+D_{j+1}^i\left(C_{j+1}^i-C_j^i\right) \tag{11}$$

(c) At the center grid point with $j = n$ and $i \geq 0$:

Due to symmetry, we can set $C_{j-1}^i=C_{j+1}^i, D_{j-1}^i=D_{j+1}^i$, and $j = n$ in Equation (11) to obtain

$$\frac{(\Delta X)^2}{\Delta t}\left(C_n^{i+1}-C_n^i\right)=D_{n-1}^i\left(C_{n-1}^i-C_n^i\right)+D_n^i\left(C_{n-1}^i-C_n^i\right) \tag{12}$$

Computational Algorithm

Suppose $C(X, \bar{t})$ and $C(X, \bar{t}+\Delta t)$ are known at evenly spaced grid points where $\bar{t}$ is specified time and Δt is time increment, and we are interested in finding the diffusion coefficient values at the grid points using the inverse method. From Equations (8), (11), and (12), we can create the following system of linear equations:

$$\mathbf{A}\,\mathbf{d}=\mathbf{b} \tag{13}$$

where **A** is an $(n+1) \times (n+1)$ matrix and **d** and **b** are $(n+1)$ vectors. **A, d,** and **b** are subscripted from 0 to n as shown below:

$$\mathbf{A}=\begin{pmatrix} a_{0,0} & a_{0,1} & & & & \\ a_{1,0} & a_{1,1} & a_{1,2} & & & \\ & \cdot & \cdot & \cdot & & \\ & & \cdot & \cdot & \cdot & \\ & & & \cdot & \cdot & \cdot \\ & & & a_{n-1,n-2} & a_{n-1,n-1} & a_{n-1,n} \\ & & & & a_{n,n-1} & a_{n,n} \end{pmatrix}$$

$$\mathbf{d}=\begin{pmatrix} D_0 \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ D_n \end{pmatrix}$$

$$\mathbf{b}=\begin{pmatrix} b_0 \\ b_1 \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ b_n \end{pmatrix} \tag{14}$$

The elements of **d** are the unknown diffusion coefficient values at the grid points, and the elements of **A** and **b** are expressed as follows:

(a) At the surface grid point with $X = X_0$ and $t = \bar{t}$:

$$a_{0,0}=(2\alpha-1)\left[C(X_0,\bar{t})-C(X_1,\bar{t})\right] \tag{15}$$

$$a_{0,1}=C(X_1,\bar{t})-C(X_0,\bar{t}) \tag{16}$$

$$b_0=\frac{(\Delta X)^2}{\Delta t}\left[C(X_0,\bar{t}+\Delta t)-C(X_0,\bar{t})\right] \tag{17}$$

(b) At an internal grid point with $X = X_j$ $(0 < j < n)$ and $t = \bar{t}$:

$$a_{j,j-1}=C(X_{j-1},\bar{t})-C(X_j,\bar{t}) \tag{18}$$

$$a_{j,j}=C(X_{j+1},\bar{t})-2C(X_j,\bar{t})+C(X_{j-1},\bar{t}) \tag{19}$$

$$a_{j,j+1}=C(X_{j+1},\bar{t})-C(X_j,\bar{t}) \tag{20}$$

$$b_j=\frac{2(\Delta X)^2}{\Delta t}\left[C(X_j,\bar{t}+\Delta t)-C(X_j,\bar{t})\right] \tag{21}$$

(c) At the center grid point with $X = X_n$ and $t = \bar{t}$:

$$a_{n,n-1}=C(X_{n-1},\bar{t})-C(X_n,\bar{t}) \tag{22}$$

$$a_{n,n}=C(X_{n-1},\bar{t})-C(X_n,\bar{t}) \tag{23}$$

$$b_n=\frac{(\Delta X)^2}{\Delta t}\left[C(X_n,\bar{t}+\Delta t)-C(X_n,\bar{t})\right] \tag{24}$$

This system consists of a tridiagonal system of linear algebric equations. The solution vector **d** is the diffusion coefficient vector. A FORTRAN subroutine based on the Thomas algorithm (Thomas 1949) can be found in Özisik (1993) for solving a tridiagonal system of equations.

A detailed error analysis of this procedure can be found in Yeung and Tam (1996) and Özisik (1993). The system of linear equations (13) is different from the original partial differential equation by an error $O[(\Delta X)^2]$,that is,

$$\mathbf{A}\,\mathbf{d}=\mathbf{b}+O[(\Delta X)^2] \tag{25}$$

which shows that the solution vector **d** has an error $O[(\Delta X)^2]$, the order of the leading error for central difference.

NUMERICAL RESULTS AND DISCUSSION

Desorption test data for northern red oak (*Quercus rubra*) by Simpson (1993) can be conveniently used for numerical analysis. The set of data selected for this study has the following specifications: (1) specimen thickness, 25 mm, (2) initial moisture content, 35.9%, (3) equilibrium moisture content, 5.5% (corresponding relative humidity, 33%), and (4) test temperature, 43.4°C. Specimens were of a parallelepiped shape and coated on four sides so that moisture could only move through the thickness, which coincides with the radial direction. Also, the test temperature had a standard deviation of 0.3°C and the relative humidity, a standard deviation of 0.7%. Moisture content is the quantity of moisture in wood expressed as a perentage of ovendry weight and is used as concentration of the diffusing substance in the diffusion equation.

The test data were fitted by a curve as shown in Figure 1, which presents the variation of moisture content with distance at t = 216.65 h. Some curve-fitted data used in the present study are shown in Figure 2.

Variations of moisture content with time at different positions are presented in Figure 3. We note that some minor shifting of the curves close to the boundary or at large times was considered necessary to make the data mathematically tractable and physically reasonable.

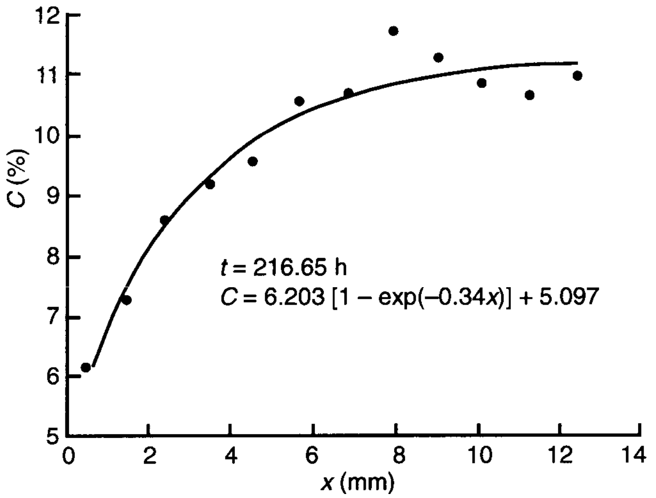

Figure 1. Moisture content as a function of distance by curve fitting.

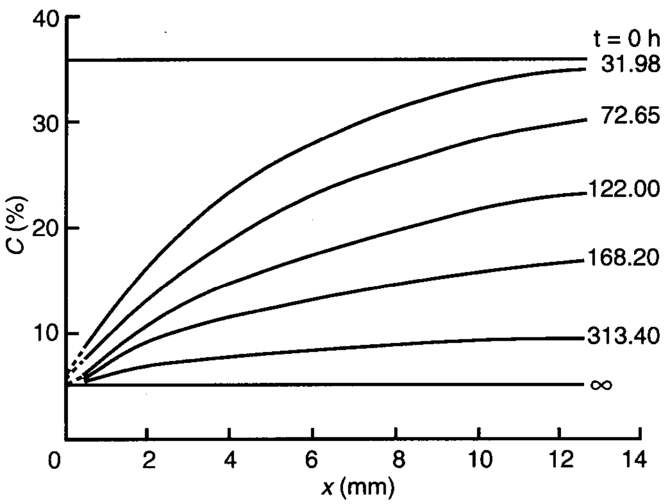

Figure 2. Moisture content as a function of distance at various times.

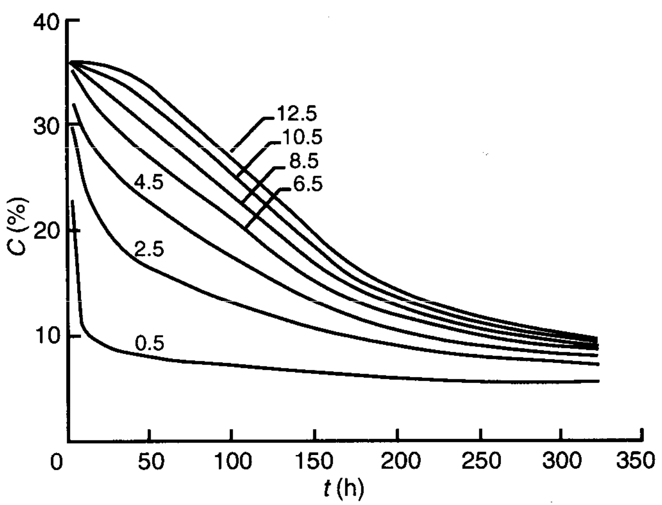

Figure 3. Moisture content as a function of time at various positions (mm).

Figure 4 presents curves of diffusion coefficient as a function of distance at different times. In the calculations, we set $\Delta X = 1$ mm and $\Delta t = 0.1$ to 0.3 h. The difference resulting from a different selection of At was found to be negligible. However, the value of a in Equations (7) and (15) was found to have a tremendous effect on the results, as shown in Figure 5. With $\alpha = 1$, the curve was found to oscillate dramatically. With $\alpha > 1$, the degree of oscillation decreased, and at $\alpha = 1.925$, the curve was found to be relatively smooth. It is of interest that the smooth curve intersected the solid line between any two adjacent points in the middle of the line. Also, at the center of a specimen where the moisture gradient is assumed to be zero, the diffusion coefficient tends to approach zero.

Variation in diffusion coefficient with moisture content at different times is displayed in Figure 6.

Our results clearly show that the diffusion coefficient varies with time, position, moisture content, and moisture gradient. The results are contrary to our original expectation, which was to find the correct dependence of the diffusion coefficient on moisture content alone. In the literature of moisture diffusion in wood, the diffusion coefficient has always been assumed to be either constant or monotonically increasing with increasing moisture content. This assumption seems to predict the moisture distribution in wood in certain situations fairly well. We are not sure whether moisture distribution in wood is only weakly dependent on the diffusion coefficient or whether the existing literature does not address the topic as comprehensively as it should.

In the present study, we used the inverse method following Chen et al. (1996) and Yeung and Lam (1996), who demonstrated the accuracy of their procedures in determining the thermal conductivity in heat conduction problems in a convincing manner. The test data by Simpson (1993), which are more comprehensive than any available to us in the literature, have also been carefully analyzed. Nevertheless, we obtained results not reported in the related literature. However, according to Crank (1975), an experimental curve relating diffusion of acetone in cellulose acetate does bear resemblance to the curves in Figure 6. The shape of the experimental curve relating diffusion of moisture in activated alumina reported by Imakoma et al. (1985) and Legros et al. (1992) is even more complex. We therefore tend to believe that our results are correct. In any case, our study clearly justifies the need for more research in this area.

CONCLUSIONS

A second-order finite difference procedure was applied for the inverse determination of the diffusion coefficient of moisture diffusion in wood. The procedure was successfully developed for the inverse determination of thermal conductivity of a one-dimensional medium. Since the governing equations for heat conduction and moisture diffusion are the same, the same solution procedure should apply to both cases.

The results indicate that the diffusion coefficient of northern red oak is a function of time, position, moisture content, and moisture gradient, which is at variance with assumptions in the related literature. However, these results seem to be similar to test data of diffusion of acetone in cellulose acetate and diffusion of moisture in activated alumina reported in the literature. Since the functional form of the diffusion coefficient of moisture diffusion in wood is generally assumed rather than experimentally determined, it seems that more research is needed in this area.

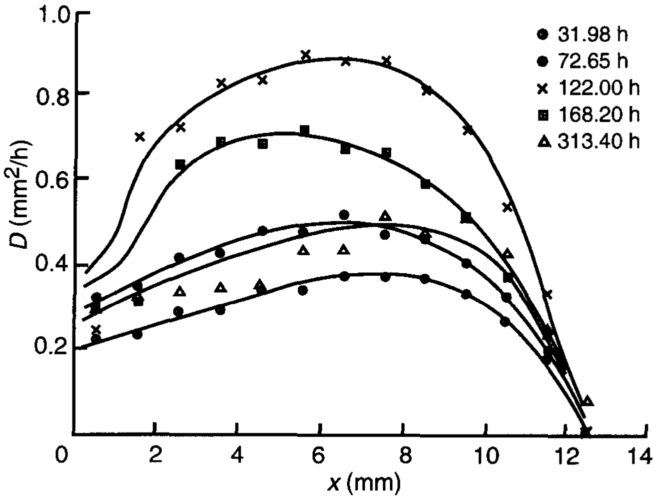

Figure 4. Diffusion coefficient as a function of distance at various times.

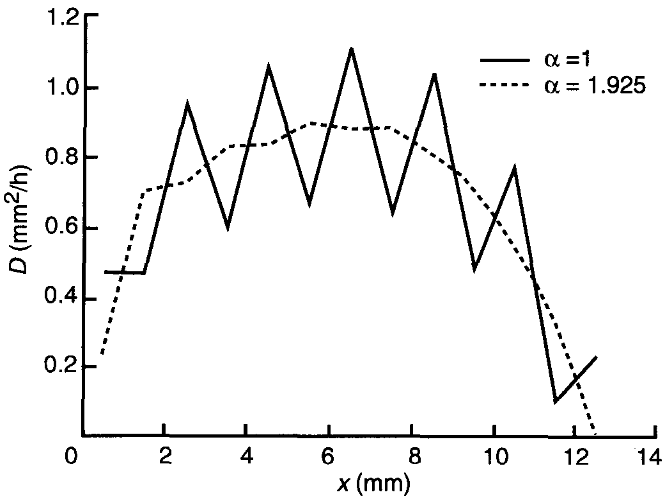

Figure 5. Effect of a on variation of diffusion coefficient with distance (t = 122 h).

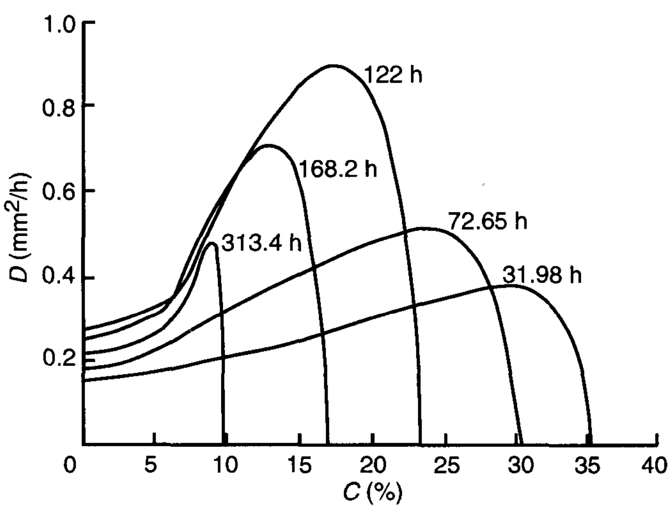

Figure 6. Diffusion coefficient as a function of moisture content at various times.

REFERENCES

Avramidis, S., and Siau, J.F., 1987, "An Investigation of the External and Internal Resistance to Moisture Diffusion in Wood," *Wood Science Technology,* Vol. 21, No. 3, pp. 249–256.

Chen, H.T., Lin, J.Y., Wu, C.H., and Huang, C.H., 1996, "Numerical Algorithm for Estimating Temperature-Dependent Thermal Conductivity," *Numerical Heat Transfer*, Part B, Vol. 29, No. 4, pp. 509–522.

Choong, E.T., and Skaar, C., 1972, "Diffusivity and Surface Emissivity in Wood Drying," *Wood Fiber,* Vol. 4, No. 2, pp. 80–86.

Crank, J.,1975, *The Mathematics of Diffusion*, Chap. 9, 2nd ed., Clarendon Press, Oxford.

Droin, A., Taverdet, J.L., and Vergnaud, J.M., 1988, "Modeling the Kinetics of Moisture Adsorption by Wood," *Wood Science and Technology,* Vol. 22, No. 1, pp. 11–20.

Hougen, C.A., McCauley, H.J., and Marshall, W.R., Jr., 1940, "Limitations of Diffusion Equations in Drying," *Trans. AIChE,* Vol. 36, pp. 183–210.

Imakoma, M., Okazaki, M., and Toei, R., 1985, "Mathematical Model for Drying of Adsorptive Porous Materials," *Acta Polytech. Scand., Chem. Incl. Metall. Ser.* , Vol. 160, pp. 1–32.

Legros,M., Imakoma, H., Yoshida, M., and Okazaki, M., 1992, "Approximate Isothermal Drying Curves of Hygroscopic Porous Materials with Given Desorption Isotherm," *Chemical Engineering and Processing,* Vol. 31, pp. 149–155.

Meroney, R.N., 1969, "The State of Moisture Transport Rate Calculations in Wood Drying," *Wood Fiber,* Vol. 1, No. 1, pp. 64–74.

Mounji, H., Bouzon, J., and Vergnaud, J.M., 1991, "Modelling the Process of Absorption and Desorption of Water in Two Dimensions(Transverse) in a Square Wood Beam," *Wood Science and Technology,* Vol. 26, No. 1, pp. 23–37.

Özisik, M.N., 1993, *Heat Conduction*, Chaps.12,14, 2nd ed., John Wiley & Sons.

Simpson, W.T., 1993, "Determination and Use of Moisture Diffusion Coefficient to Characterize Drying of Northern Red Oak," *Wood Science and Technology,* Vol. 27, No. 6, pp. 409–420.

Skaar, C., 1954, "Analysis of Methods for Determining the Coefficient of Moisture Diffusion in Wood," *Journal of Forest Products Research Society,* Vol. 4, No. 6, pp. 403–410.

Soderström, O., and Salin, J.G., 1993, "On Determination of Surface Emission Factors in Wood Drying," *Holzforschung,* Vol. 47, No. 5, pp. 391–397.

Thomas, L.H., 1949, *Elliptic Problems in Linear Difference Equations Over a Network*, Watson Scientific Computer Laboratory Report, Columbia University, New York.

Van Arsdel, W.B., 1947, "Approximate Diffusion Calculations for the Falling Rate Phase of Drying," *Trans. AIChE,* Vol. 43, pp. 13–24.

Yeung, W.K., and Lam, T.T., 1996, "Second-Order Finite Difference Approximation for Inverse Determination of Thermal Conductivity," *International Journal of Heat Mass Transfer,* Vol. 39, No. 17, pp. 3685–3693.