EVALUATION OF DIFFUSION COEFFICIENT AND SURFACE EMISSION COEFFICIENT BY AN OPTIMIZATION TECHNIQUE[1]

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ABSTRACT

The rate at which wood dries can be expressed by two factors: (1) the diffusion coefficient, as an indication of internal resistance to moisture removal, and (2) the surface emission coefficient, as an indication of external resistance to moisture removal. An optimization technique was applied to calculate these two coefficients. Unlike existing methods where these coefficients are evaluated at only one point, usually at one-half of the evaporable water remaining in wood, this optimization technique used the entire drying data. The technique searches for the optimum pair of coefficients based on the least squares principle. The performance of this method was demonstrated by reanalyzing published data using a digital computer. The results indicate that a more accurate prediction of the drying process can be achieved by the optimization method than by existing methods. The dependence of the diffusion coefficient on moisture content and sample thickness is discussed.

Keywords: Diffusion coefficient, surface emission coefficient, optimization, conjugate gradient.

INTRODUCTION

The diffusion coefficient in wood determines the rate of internal moisture movement, while the surface emission coefficient describes the rate at which moisture is emitted from the surface of drying wood. Methods to evaluate

these two coefficients in wood drying practice have been studied extensively since Skaar (1954) introduced Newman's general solution (Newman 1931) of the unsteady-state diffusion equation into the field of wood drying. Based on a graphical solution of Newman's equation, Choong and Skaar (1969) suggested an approximate method to evaluate the diffusion coefficient, D, and the surface emission coefficient, S. According to this method, D and S can be calculated if the drying times for two samples with different thicknesses are known

for reduction of the fractional moisture content (MC) $\bar{E}$ in wood to 0.5. Later, Choong and Skaar (1972) developed a more general form to enable D and S to be calculated from simultaneous drying experiments on samples of several different thicknesses. Using the same analytical procedure, Rosen (1978) proved that air velocity had a significant influence on the surface emission coefficient related to the external resistance in the sorption process. He found that the relative importance of external resistance to moisture movement in wood increased as specimen thickness and/or air velocity decreased. Liu (1989) described a modified method based on Choong and Skaar's (1969) approach to estimate D and S from a single lumber-drying curve. His method requires knowledge of both the drying time and the slope of the fractional moisture content-drying time curve at $\bar{E} = 0.5$.

There are two common characteristics for the above approximate methods. First, the calculations are carried out at one point, $\bar{E} = 0.5$. Second, the resulting diffusion coefficient and surface emission coefficient are assumed to be constant, independent of $\bar{E}$. If the final aim is to predict accurately the experimental data over the entire drying period, the pair of coefficients evaluated at $\bar{E} = 0.5$ may not be the ideal ones since the diffusion coefficient is generally not constant but a function of wood MC (Comstock 1963; Stamm 1964; Choong 1965). There were no published data available to describe how well the pair evaluated at $\bar{E} = 0.5$ compared with those evaluated at other values of $\bar{E}$.

The objectives of this study were: 1) to search the best pair of diffusion coefficients and surface emission coefficients by using an optimization technique based on the least squares principle and Newman's general theoretical solution, 2) to evaluate how the variation of diffusion coefficients with MC affects the predictability of the drying curve.

BASIC EQUATIONS AND OPTIMIZATION PROCEDURE

The general partial differential equation for unsteady-state moisture diffusion in the direction perpendicular to the surface can be expressed by Fick's second law:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial X}\left(D\frac{\partial C}{\partial X}\right) \qquad (1)$$

where C is moisture concentration (or MC), t time, X distance from the centerline, and D the diffusion coefficient, which is a function of moisture concentration.

Initial and boundary conditions for moisture evaporation at the surface are given by

$$C = C_0, \quad -a < X < a, \qquad t = 0 \qquad (2)$$

and

$$\pm D\frac{\partial C}{\partial X} = S(C_e - C_a), \quad X = \pm a, \qquad t \geq 0 \qquad (3)$$

where C_e is the moisture concentration in equilibrium with the water vapor pressure in the surrounding air, C_a the actual moisture concentration in the surface at any time, a the half-thickness of the specimen, and S the surface emission coefficient.

If D is a constant, a theoretical solution for Eq. (1), as given by Newman (1931), is:

$$\bar{E} = \frac{\bar{C} - C_e}{C_0 - C_e} = 2L^2 \sum_{n=1}^{\infty} \frac{\exp(-\beta_n^2\tau)}{\beta_n^2(\beta_n^2 + L^2 + L)} \qquad (4)$$

where $\bar{C}$ is the average value of C across the specimen thickness, β_n are the positive roots of

$$\beta_n\tan \beta_n = L \qquad (5)$$

where

$$L = Sa/D, \qquad (6)$$

and

$$\tau = Dt/a^2. \qquad (7)$$

Since the diffusion coefficient in wood during drying is generally a function of the moisture concentration, the D calculated from Eq. (4) represents some average value over the concentration range.

In the present work, we take the alternate approach of searching for an optimum pair of constants, D and S, which minimize the sum
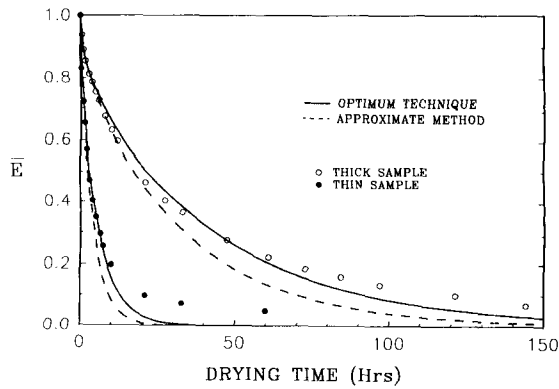
FIG. 1. Drying curves from the optimization technique and the approximate method. (Data from Choong and Skaar 1969.)

of squares of the differences between experimental data and Eq. (4). To fulfill this task, an ascent optimization algorithm was applied. The search can begin from any reasonable pair of D and S values. After each iteration, a new D and S pair with a smaller sum of squares is obtained. Finally, the search stops after the reduction in the sum of squares from one iteration to the next is less than the given closure criterion. A FORTRAN program was written to accommodate the calculation. In this program, a bisection technique is employed to guarantee accurately finding all positive roots in Eq. (5) for any L. A conjugate gradient technique is used to increase the climbing speed toward the minimum absolute value of Negative Mean Sum of Squares (NMSS), which is defined as $-\Sigma \, (\Delta\bar{E})^2/N$, where $\Delta\bar{E}$ is the difference in the fractional moisture content between the fitted curve and the experimental data and N is the number of data points. When the optimum pair of D and S has been found, the corresponding drying curve can be computed from Eq. (4).

NUMERICAL EXAMPLE AND DISCUSSION

Choong and Skaar (1969) evaluated the D and S at $\bar{E} = 0.5$ using their approximate method for yellow-poplar sapwood and heartwood specimens, dried in both the tangential and the

radial directions. Two samples of different thicknesses were dried for each combination in an environmental chamber at 32 ± 0.2 C and 40% relative humidity at an air speed of 3.3 m/sec. Their results for sapwood in the tangential direction were $D = 7.5 \times 10^{-10}$ m^2/sec and $S = 1.52 \times 10^{-6}$ m/sec. Similar results were obtained by Liu (1989) using one sample and the slope technique. The data for sapwood in the tangential direction were chosen for the evaluation of D and S in the present study.

The predicted drying curves (dashed lines) from the approximate D and S above are shown in Fig. 1. Since they are based on data at $\bar{E} = 0.5$, the approximate techniques fit well at that point, but poorly elsewhere. The calculated drying curves seriously underpredict the drying time necessary to reach lower $\bar{E}$ values. The application of the optimization technique significantly enhanced the predictability of the experimental data. The solid $\bar{E}$ curves (Fig. 1) are those that correspond to the optimum S and D using the entire drying data in accordance with minimum NMSS criterion. The absolute values of the NMSS by the two approximate methods shown in Table 1 (Choong and Skaar 1969; Liu 1989) were more than 3.4–3.6 times larger than those resulting from the optimization technique for the thick and thin samples, respectively.

The relationship of the optimum $\bar{E}$ curves to the experimental data (Fig. 1) indicates that the diffusion coefficient was a function of MC. For both thick and thin samples, the experimental $\bar{E}$ data are located below the optimum $\bar{E}$ curve in the higher MC range and above it in the lower MC range, suggesting that the diffusion coefficient decreased with a reduction in MC. This is consistent with similar findings by Comstock (1963) and Choong (1965). To confirm this point more quantitatively, an extension of the optimization procedure was carried out by calculating a series of D and S pairs over reduced moisture ranges, using the same final MC. As shown in Table 1, the optimum diffusion coefficient tended to decrease gradually with a decrease in average MC. For the surface emission coefficient, the thick sample

TABLE 1. *Comparison of Values[a] of S, D, and NMSS from the optimization technique with those from two approximate methods over the reduced moisture ranges for the thick and thin samples.*

Method	MC range from $\bar{E} = 1$ to $\downarrow$	S (m/sec)	D (m²/sec)	NMSS data
		Thick sample (half-thickness = 14.31 mm)		
Approximate 1[b]		1.52N6	7.50N10	−2.78N3
Approximate 2[c]		1.48N6	7.35N10	−2.47N3
Optimization	0.89	1.43N6	8.95N10	−5.40N2
	0.86	1.74N6	7.65N10	−1.11N6
	0.82	2.21N6	6.81N10	−3.03N6
	0.79	2.67N6	6.39N10	−4.81N6
	0.75	2.39N6	6.60N10	−5.18N6
	0.73	2.30N6	6.67N10	−4.63N6
	0.68	2.07N6	6.87N10	−5.75N6
	0.63	2.02N6	6.91N10	−5.23N6
	0.60	2.01N6	6.92N10	−4.71N6
	0.46	2.32N6	6.72N10	−7.63N6
	0.40	3.08N6	6.43N10	−2.34N5
	0.37	5.13N6	6.12N10	−6.52N5
	0.28	2.52N5	5.79N10	−1.42N4
	0.22	>0.40	5.62N10	−2.46N4
	0.18	>0.40	5.51N10	−3.57N4
	0.16	>0.40	5.41N10	−4.84N4
	0.13	>0.40	5.33N10	−5.89N4
	0.10	>0.40	5.28N10	−6.87N4
	0.07	>0.40	5.25N10	−7.22N4
		Thin sample (half-thickness = 4.79 mm)		
Approximate 1[b]		1.52N6	7.50N10	−4.69N3
Approximate 2[c]		1.66N6	7.14N10	−4.25N3
Optimization	0.72	>0.40	4.61N10	−5.88N6
	0.65	>0.40	4.61N10	−3.97N6
	0.57	>0.40	4.60N10	−3.00N6
	0.47	1.12N4	4.66N10	−6.36N6
	0.40	1.05N4	4.67N10	−5.30N6
	0.35	>0.40	4.57N10	−3.62N5
	0.29	>0.40	4.50N10	−8.90N5
	0.26	>0.40	4.43N10	−1.37N4
	0.20	>0.40	4.34N10	−3.26N4
	0.10	>0.40	4.29N10	−7.64N4
	0.07	>0.40	4.28N10	−1.08N3
	0.05	>0.40	4.28N10	−1.16N3

[a] The notation xNy means $x \times 10^{-y}$
[b] Values of S, D are from Choong and Skaar (1969).
[c] Values of S, D are from Liu (1989).

and the thin sample seemed to follow somewhat different trends. In the thick sample, the definite values of S could be searched out over the relatively high moisture ranges; but they became very large (>0.40 m/sec) when the relatively low moisture ranges were reached. In the thin sample, the definite values of S could be searched out only at the medium moisture ranges; and the values of S were very large

(<0.40 m/sec) at rather high and low moisture ranges; thus the sample thickness could also be an affecting variable.

The diffusion coefficient may depend on the sample thickness. The optimum D for the thin sample is 18% smaller than for the thick sample (Table 1). A similar result was reported by Choong and Skaar (1969, 1972), who explained that the discrepancy in the "apparent"

diffusion coefficients was due to a change in the external resistances of samples of different thicknesses. However, their air speed was 3.3 m/sec, which is greater than the threshold value of 3.0 m/sec (Rosen 1978) above which the external resistance is negligible. Therefore, other factors such as a time-dependent deformation of the cellulose-lignin matrix (Hart 1964) and drying stress could contribute to this discrepancy.

CONCLUSIONS

The optimum values of the diffusion coefficient and surface emission coefficient can be determined from a single drying curve using an optimization technique. This technique gives a more accurate prediction of experimental data than existing approximate methods. In a typical drying case, the diffusion coefficient was found to be a function of moisture content as well as sample thickness.

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