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AN INVERSE MOISTURE DIFFUSION ALGORITHM FOR THE DETERMINATION OF DIFFUSION COEFFICIENT

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ABSTRACT

The finite difference approximation is applied to estimate the moisture-dependent diffusion coefficient by utilizing test data of isothermal moisture desorption in northern red oak *(Quercus rubra)*. The test data contain moisture distributions at discrete locations across the thickness of specimens, which coincides with the radial direction of northern red oak, and at specified times. Also, the rate of moisture variation at each specified time and location must be known or correctly estimated. The functional form of the diffusion coefficient as well as the boundary conditions at the surfaces are not known *a priori*. The resulting system of finite difference equations defines an inverse problem, whose solution may be sensitive

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to small changes of input data. Results indicate that the diffusion coefficient increases with increasing moisture content below the fiber saturation point, which defines the upper limit applied by the diffusion theory.

Key Words: Desorption; Inverse method; Moisture; Wood

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). The test data moisture distributions at discrete locations across the thickness of specimens, which coincides with the radial direction of northern red oak, and at specified times. To reduce the effects of data scatter, the test data were simulated by mathematical modeling. The simulated data represent the test data very close and were analyzed using the finite differences technique. Results indicate that the diffusion coefficient increases with increasing moisture content below the fiber saturation point. The diffusion coefficient increases dramatically when moisture content is low and tends to level off as moisture content approaches the fiber saturation point (see Figure 6).

In solving the diffusion equation for moisture variations 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 al. 1991, Soderström and Salin 1993). Also, different boundary conditions have been assumed by different authors (e.g., Crank 1975, Plumb et al. 1985, Salin 1996, Hukka 1999). No one has ever attempted to use the inverse method to verify assumptions. In using the inverse method, the governing partial differential equation is converted into a system of linear equations based on test data; the boundary conditions need not be specified in the formulation. In the system of linear equations, the unknowns are the values Of the diffusion coefficient corresponding to different moisture content values, locations, and times, which can be easily obtained. The advantage of this approach, is that no prior information or assumption required on either the functional form of the diffusion coefficient or the exact mechanism of surface evaporation in diffusion. Once the diffusion coefficient values have been determined, the corresponding boundary condition can be evaluated.

The inverse method has been used successfully to 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 desoption process of wood. The only condition for such an application is that moisture variations with time and space in wood be known over the entire domain of interest; for northern red oak, these moisture values are available in the work of Simpson (1993).

The inverse solutions are known to be 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* or *ill-conditioned* problems; that is, their solutions do not satisfy the general requirements of existence, uniqueness, and stability under small changes to the input data (Özisik 1993). In the present study, the time derivative of the diffusion equation must be approximated with special care as the time intervals for data collection were relatively large, making it difficult for precise time derivative estimation. However, in spite of the uncertainties, our results have demonstrated the special merits of the solution procedure.

ONE-DIMENSIONAL ISOTHERMAL DIFFUSION EQUATIONS

In a one-dimemional formulation with moisture moving in the direction normal to a specimen of a slice of wood of thickness 2a, the diffusion equation can he written as

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

where C is moisture content, t is time, D is diffusion coefficient, and X is space coordinate measured from the center of the specimen.

Let the initial condition be

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

where C_0 is a constant moisture content in the specimen, and let the boundary conditions be

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

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

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

The 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 points, as described in the next section. Note that Equation (4) is listed for reference only. It is not needed in solving for $D(X, t)$ in the present work.

INVERSE DETERMINATION OF DIFFUSION COEFFICIENT

First, we present a finite difference procedure for calculating the diffusion coefficient at discrete grid points. Then, we give the computational algorithm for determining the diffusion coefficient values corresponding to different times and positions.

Finite Difference Formulation

Let half of specimen thickness (a) be discretized with mesh width (ΔX) in space (Figure 1b) and Δt 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 = 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 the forward difference to the time derivative of Equation (1) yields

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

and applying the forward difference to the space derivative yields

$$\begin{aligned}\left[\frac{\partial}{\partial X}\left(D\frac{\partial C}{\partial X}\right)\right]_0^i &= \left[D\frac{\partial^2 C}{\partial X^2} + \frac{\partial D}{\partial X}\cdot\frac{\partial C}{\partial X}\right]_0^i \\ &\cong \left[D_0\frac{C_2 - 2C_1 + C_0}{(\Delta X)^2} + \frac{D_1 - D_0}{\Delta X}\cdot\frac{C_1 - C_0}{\Delta X}\right]_0^i \\ &= \frac{1}{(\Delta X)^2}\left[D_1^i(C_1^i - C_0^i) + D_0^i\cdot(C_2^i - 3C_1^i + 2C_0^i)\right]\end{aligned} \tag{6}$$

Equating Equations (5) and (6) gives

$$\frac{(\Delta X)^2}{\Delta t}(C_0^{i+1} - C_0^i) = D_0^i(C_2^i - 3C_1^i + 2C_0^i) + D_1^i(C_1^i - C_0^i) \tag{7}$$

We avoided using Equation (4) by applying forward difference to the space derivative in Equation (6).

b. At an internal grid point $0 < j < n$ and $i > 0$,

$$\left(\frac{\partial C}{\partial t}\right)_j^i = \frac{C_j^{i+1} - C_j^i}{\Delta t} \tag{8}$$

and

$$\left[\frac{\partial}{\partial X}\left(D\frac{\partial C}{\partial X}\right)\right]_j^i = \left[D_j\frac{C_{j+1} - 2C_j + C_{j-1}}{(\Delta X)^2} + \frac{D_{j+1} - D_{j-1}}{2\Delta X}\cdot\frac{C_{j+1} - C_{j-1}}{2\Delta X}\right]_j^i \tag{9}$$

Equating Equations (8) and (9) yields

$$\frac{4(\Delta X)^2}{\Delta t}\cdot(C_j^{i+1} - C_j^i) = D_{j-1}^i(C_{j-1}^i - C_{j+1}^i) + 4D_j^i(C_{j+1}^i - 2C_j^i + C_{j-1}^i) + D_{j+1}^i(C_{j+1}^i - C_{j-1}^i) \tag{10}$$

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 (10) to obtain

$$\frac{(\Delta X)^2}{\Delta t}(C_n^{i+1} - C_n^i) = 2D_n^i(C_{n-1}^i - C_n^i) \tag{11}$$

Computational Algorithm

Suppose $C(X, \bar{t})$ and $C(X, \bar{t}, + \Delta t)$ are known at evenly spaced grid points where t is specified time and Δt is time increment, and we are interested in finding the diffusion coefficient values at the grid points. From Equations (7), (10) and (11), we can derive the following system of linear equations:

$$\mathbf{Ad=b} \tag{12}$$

where **A** is an $(n + 1) \times (n + 1)$ matrix and **d** and **b** are $(n + 1)$ vectors. The solution is

$$\mathbf{d=A^{-1}b} \tag{13}$$

where A^{-1} is inverse of A. Equation (12) defines a relatively simple inverse problem (Hensel 1991). **A**, **d**, and **b** are subscripted from 0 to n as shown below:

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

$$\mathbf{d} = \begin{bmatrix} D_0 \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ D_n \end{bmatrix} \quad \mathbf{b} = \begin{bmatrix} b_0 \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ b_n \end{bmatrix} \tag{14}$$

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

a. At the surface grid point with $X = X_0$ and $t = \bar{t}$,

$$a_{0,0} = 2C(X_0,\bar{t}) - 3C(X_1,\bar{t}) + C(X_2,\bar{t}) \tag{15}$$

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

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

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

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

$$a_{j,j} = 4\left[C(X_{j+1},\bar{t}) - 2C(X_j,\bar{t}) + C(X_{j-1},\bar{t})\right] \tag{19}$$

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

$$b_j = \frac{4(\Delta X)^2}{\Delta t}\left[C(X_j,\bar{t} + \Delta t) - C(X_j,\bar{t})\right] \tag{21}$$

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

$$a_{n,n} = 2\left[C\left(X_{n-1},\bar{t}\right) - C\left(X_n,\bar{t}\right)\right] \tag{22}$$

$$b_n = \frac{(\Delta X)^2}{\Delta t}\left[C\left(X_n,\bar{t}+\Delta t\right) - C\left(X_n,\bar{t}\right)\right] \tag{23}$$

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

The system of linear equations (Eq. 12) is different from the original partial differential equation (Eq. 1) because of the finite difference approximation. Also, as described in Hensel (1991), a small change in vector **b** may result in large changes in the solution vector **d,** depending on the degree of the "ill-conditioning" property of matrix. A. Therefore, the importance o accurate data generation cannot be overemphasized in applying the inverse technique.

NUMERICAL RESULTS AND DISCUSSION

Desorption test data for northern red oak by Simpson [1] can be conveniently used for numerical analysis. The set of data selected for this study has the following specifications: (1) specimen thickness, 2a, 25 mm, (2) initial moisture content, C_0, 35.9%, (3) equilibrium moisture content C_e , 5.5% (corresponding relative humidity, 33%), and (4) test temperature, 43.4°C. Specimens were taken from flat-saw boards as right parallelepipeds and coated on four sides with two coats of heavily pigmented aluminum paint so that moisture could move only through the thickness, which coincides nominally with the radical direction (Figure 1a). This configuration chosen because the log was not large enough to ignore growth ring curvature through the thickness of the specimen. Also, the standard deviation of the test temperature was 0.3°C and that of the relative humidity, 0.7%. Moisture content is the quantity of moisture in wood expressed as a percentage of ovendry weight.

The test data were fitted by a curve as shown in Figure 2, which presents the variation of moisture content with space at t = 216.6 h. Some curve-fitted data used in the study shown Figure 3.

Variations of moisture content with time at different positions are presented in Figure 4. Note that these curves were plotted with limited data in the time axis. In estimating the elements in vector **b** for a small value of Δt, these curves need to be approximated mathematically on a

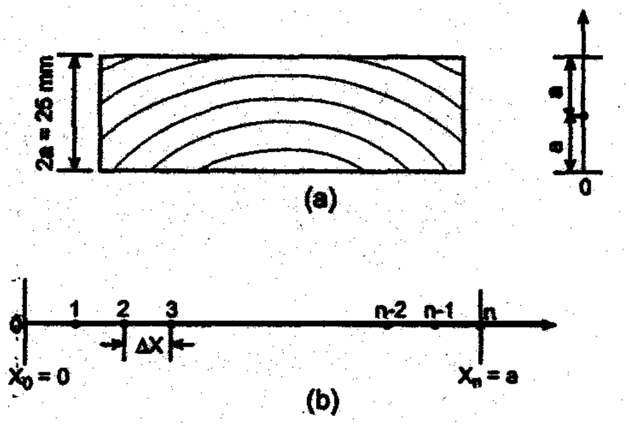

Figure 1. Test specimen and discretization of space co-ordinate. (a) Specimen with thickness in radial direction; (b) discretization of space coordinate with mesh width.

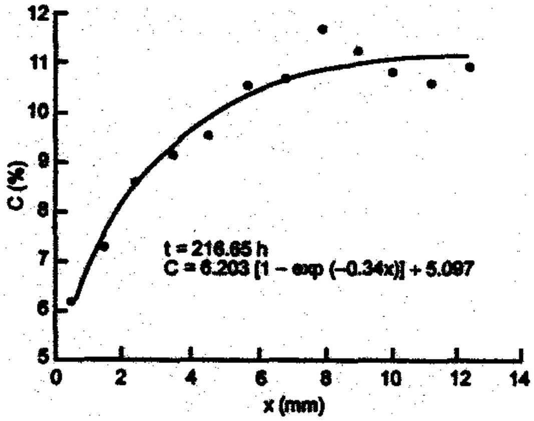

Figure 2. Moisture content as a function of space by curve fitting.

sectional basis because data extrapolation rather than interpolation may become necessary for large time intervals.

Figure 5 presents data of variations of diffusion coefficient as a function of space at different times. In the calculations, we set DX = 1 mm and Δt = 0.1 to 0.3 h. The difference resulting from a different selection of At was found to be negligible. For $t \geq$ 122h, the data tended to move in a. zigzag pattern in the central portion of the figure. This was also observed by Yeung and Lam (1996) in on of their examples, without an explanation

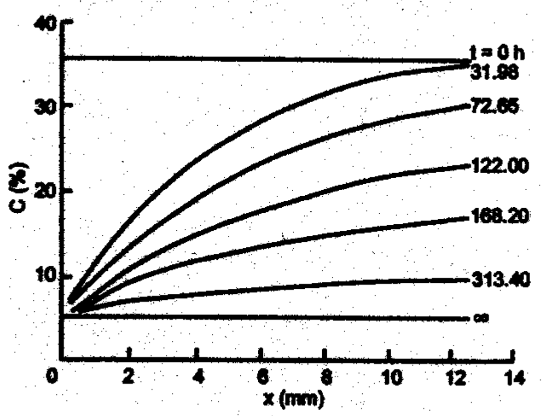

Figure 3. Moisture content as a function of space at various time points.

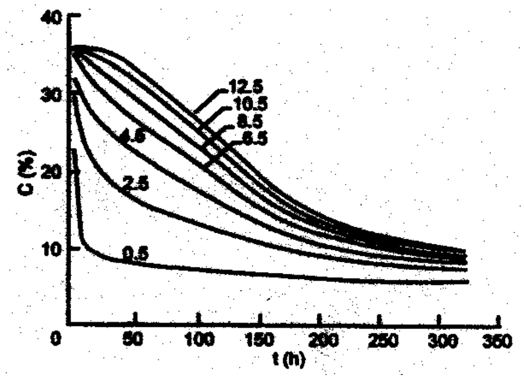

Figure 1. Moisture content as a function of time at various positions (mm).

Since their examples were problems with known analytical solutions, the observed pattern could not be due to experimental uncertainty. As pointed out previously in this paper, Equation (12) is ill-conditioned and the solution vector **d** depends on the ill-conditioning property of matrix **A;** therefore, we suspect the zigzag pattern in Figure 5 could reflect this property of matrix **A** (Hensel 1991). Close to the center of a specimen where the moisture gradient tends to approach zero, the diffusion coefficient drops to a small value in all area.

Variation in diffusion coefficient with moisture content at different times is displayed in Figure 6. If we ignore the data that fall on an imaginary curve dropping downward for each specified time and the data depicting the

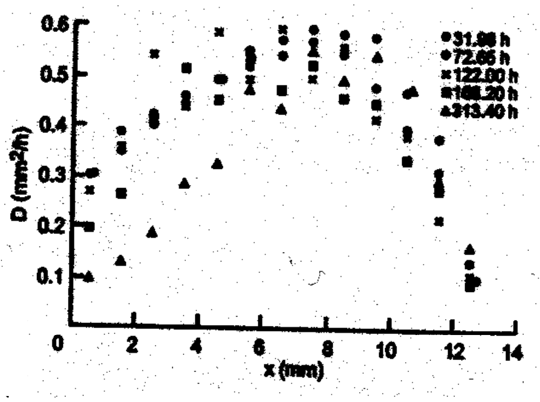

Figure 5. Variations of diffusion coefficient with space at various time points.

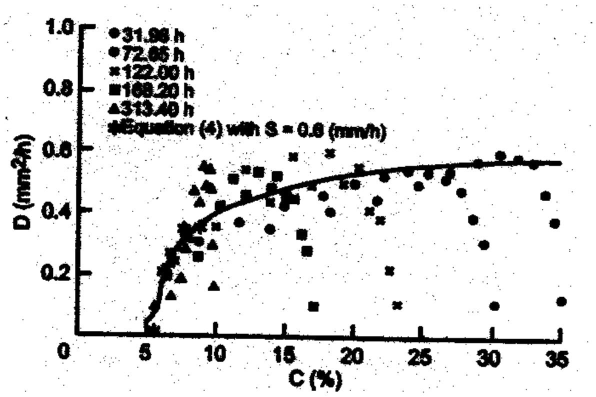

Figure 6. Variations of diffusion coefficient with moisture content at various time points.

peaks of the zigzag portions, the remaining data can be represented by the solid curve. The data dropping downward present data close to the center of a specimen, where D, being coupled with $\partial C/\partial X$ in Equation (1), can take any finite value without affecting the final results. For the zigzag portions, a peak and adjacent valley are separated by 1 mm in space in Figure 5; we have selected the valleys, which stay closer to the other data points, to obtain the solid curve in Figure 6.

The solid curve therefore defines the approximate relationship between the diffusion coefficient and the moisture content for all cases. Note that the solid curve can be obtained from the data at one small specified time only, if the data were very accurate. Also note the that at large times, the data tend to be sporadic and are unreliable. Therefore, in applying the inverse method, it is more important to have a small amount of reliable data collected at small times than a large amount of unreliable data collected at large times. In the ideal situation, the numerical approach should yield the results in Figure 7, where the solid line is the solution curve and the broken lines are to be replaced by their vertical projections on the solid line.

Figure 6, also contains a point for each specified time based on Equation (4). These points correspond to a surface emission coefficient of S = 0.6 mm/h. While Equation (4) may be controversial physically (Salin 1996, Hukka 1999), it does match the numerical results of the study reported here very closely.

Figure 8 compares the solution we with the curve by Simpson (1993). Except for small values of moisture content, the two curves follow

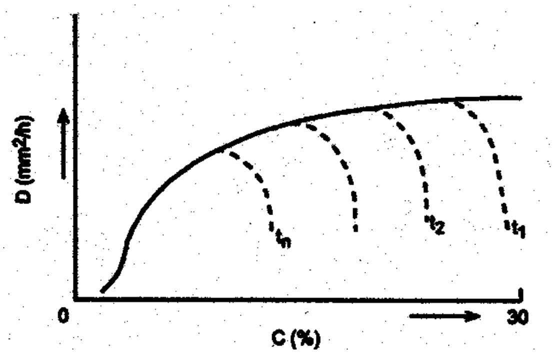

Figure 7. Ideal variations of diffusion coefficient with moisture content at various time points ($t_1 < t_2 ... < t_n$).

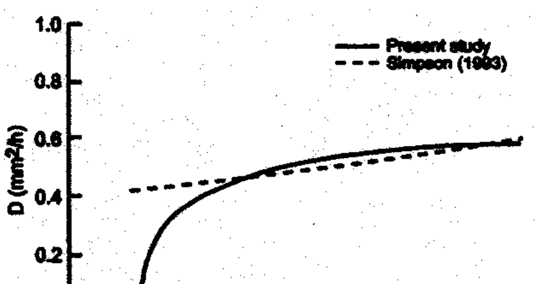

Figure 8. Comparison of diffusion coefficient variation with moisture content.

each other very closely. Note that in the calculations by Simpson (1993), the surface moisture content was assumed to be equal to the equilibrium moisture content C_e at all times; that is, S was assumed to be infinity in Equation (4).

In the present, we used the inverse method following Chen et al., (1996) and Yeung and Lam (1996), who demonstrated the accuracy of their numerical in determining the thermal conductivity in heat conduction problems, to solve our moisture diffusion problems. The test data of moisture desorption in wood by Simpson (1993), which are more comprehensive than any available to us in the literature, have been used in the analysis. The time derivative in the diffusion equation can only be approximated and may contain some uncertainties. We tried to use the Laplace transform with respect to time t in Equation (12) to solve the problem (Chen et al., 1996), but it proved to be too time-consuming. Since our existing test data were not tailored for the numerical technique in both material selection and data collection, we decided to follow the relatively simple approach with the purpose of elucidating the merits of the inverse method. To that end, we have achieved seasonable success. The technique demonstrated should provide a powerful tool in our efforts to study the problem of moisture diffusion in wood.

CONCLUSIONS

A finite difference procedure was applied for the inverse determination of the diffusion coefficient for moisture diffusion in wood.
The procedure has the following advantages:

1. The functional form of the diffusion coefficient is not known *a priori*
2. The boundary condition need not be specified.
3. Only a small amount of accurate data collected within a short period of time is needed

The disadvantages are:

1. Log selection and specimen preparation require relatively high accuracy; e.g., interference of ring curvature must not be excessive, and direction of moisture movement most be well defined.
2. Data collection technique must be sophisticated so that time derivative of moisture content at a specified time and space can be correctly estimated.

Results indicate that for northern red oak, the diffusion coefficient is a function of moisture content only. It increases dramatically at low moisture content and tends to level off as the fiber saturation point is approached. Also, the boundary condition defined in Equation (4) seems to match the results very well.

NOTATION

a	Half specimen thickness	mm
A	Matrix	
b	Vector	
C	Moisture content	%
d	Vector	
D	Diffusion coefficient	mm^2/h
S	Surface emission coefficient	mm/h
t	Time	h
X	Space	mm

Subscripts

e	Equilibrium
0	Initial, surface

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