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Estimations of Moisture Profiles during Wood Drying Using an Unsteady-State Diffusion Model (I)[*1]

- Numerical Solution -

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非定常 狀態의 擴散 모델을 이용한 水分傾斜의 豫測 (I)[*1]

- 數値解析 -

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요 약

木材의 乾燥過程 중에 발생하는 목재 내부의 水分傾斜를 예측하기 위해 非定常狀態의 擴散모델을 支配方程式으로 적용하였으며, 목재 표면에서의 蒸發抵抗과 내부의 대칭적 수분분포를 境界條件으로 채택하였다. 주어진 경계조건에서의 지배방정식에 대한 一般解가 무한수열 형태로 이루어지기 때문에, 有限差分法을 이용하여 數値解析하였으며, 有限差分法 중 誤差範圍가 안정한 상태인 Crank-Nicolson Scheme 알고리즘을 채택하였다.

Keywords : Wood drying, unsteady state diffusion, moisture gradients, finite difference method, Crank-Nicolson scheme

1. INTRODUCTION

The drying of wood is a complex process involving simultaneous transfer of heat and mass in a multi-phase system. In coupled heat and mass transfer, the flux of moisture is related to both the gradient of moisture concentration and temperature which is called the "Soret effect" (Briggs, 1967). Under isothermal conditions, Fick's second law of diffusion has been widely applied to characterize the drying behavior of wood during unsteady state moisture transfer. The application of this model is, however, limited to certain concentration ranges, such as the hygroscopic range of wood moisture content. Therefore the application of the model to wood drying over the entire range of moisture content needs several theoretical assumptions as reference levels such as the continuity of moisture gradients throughout the drying process, and the similarities of temperature dependent diffusion coefficients between the well above and below the Fiber Saturation Point(FSP) as discussed by Stamm(1964).

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A closed form solution of Fick's diffusion equation, as a governing equation with boundary conditions, gives a form of infinite series which causes tedious work in manipulating the moisture distribution for a given geometry. An attractive alternative would use numerical approximations, and a comprehensive method is thus introduced in this research. Derivative type boundary condition at the surfaces of wood is employed with the governing equation. Numerical solution is employed with a new algorithm using the finite difference method and the so called "Crank-Nicolson Scheme."

2. MATHEMATICAL BACKGROUND

2.1 Diffusion Equations

For a system of coupled heat and mass transfer under pressure differential, the differential equation for mass transfer will be of the form :

$$\frac{\partial u}{\partial \tau} = K_{21} \nabla^2 T + K_{22} \nabla^2 u + K_{23} \nabla^2 P \quad \cdots\cdots (1)$$

where u, T, P are mass content, temperature and total pressure of a body, and K_{ij} are thermodynamics coefficients(Luikov, 1966). If during mass transfer the body temperature and pressure are constant, T, P=constant($\partial T/\partial \tau = 0$; $\nabla T = 0$; $\nabla^2 P = 0$; $\partial T/\partial \tau = 0$; $\nabla P = 0$; $\nabla^2 P = 0$), the classical Fick's diffusion equation is obtained:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial X}\left(D \frac{\partial C}{\partial X}\right) \quad \cdots\cdots (2)$$

where C is a concentration, t is time(sec.), X is a space of the geometry(cm), and D is a diffusion coefficient(cm^2/sec.). The governing equation states that the rate of moisture movement is proportional to the product of the diffusion coefficient and the moisture gradient. The ground work of mathematical modeling for the drying of solids using Equation(2) has been performed since Newman(1931).

2.2 Closed Form Solution of Diffusion Equation

The analytical solution of Equation(2) can be obtained by either separation of variables or Laplace transformation(Crank, 1975) for the constant diffusion coefficient case with boundary conditions. If the region $-a \leq X \leq +a$, where a is the half thickness of a board, is initially at a uniform concentration C_0, and surfaces are kept at a constant concentration C_1, the solution of Equation(2) becomes:

$$\frac{C - C_0}{C_1 - C_0} = 1 - \frac{4}{\pi} \sum_{n=0}^{\infty} \exp \frac{-D(2n+1)^2 \pi^2 t}{4a^2} \cos \frac{(2n+1)\pi X}{a^2} \quad \cdots\cdots (3)$$

By integrating both sides of Equation(3) over the half thickness of the slab in terms of average moisture content, M, Equation(3) becomes:

$$\frac{M - M_e}{M_i - M_e} = \frac{8}{\pi^2} \sum_{n=0}^{\infty} \frac{1}{(2n+1)^2} \exp \frac{-D(2n+1)^2 \pi^2 t}{4a^2} \quad \cdots\cdots (4)$$

where M_e and M_i are equilibrium and initial moisture content. Another analytical solution of Equation(2) from Boltzmann's transformation, which is useful for small time periods, is :

$$\frac{C - C_0}{C_1 - C_0} = \sum_{n=0}^{\infty} (-1)^n erfc \frac{(2n+1)a - x}{2\sqrt{Dt}} + \sum_{n=0}^{\infty} (-1)^n erfc \frac{(2n+1)a + x}{2\sqrt{Dt}} \quad \cdots\cdots (5)$$

and the corresponding expression in terms of average moisture content is:

$$\frac{M - M_e}{M_i - M_e} = 2\sqrt{\frac{Dt}{a^2}} \left(\frac{1}{\sqrt{\pi}} + 2\sum_{n=0}^{\infty} (-1)^n ierfc \frac{na}{\sqrt{Dt}}\right) \quad \cdots\cdots (6)$$

where $erfc(z)$ is defined as $1\text{-}erf(z)$, and $erf(z)$

is the error function as a standard mathematical function, and $ierfc(z)$ is the integration of $erf(z)$ function.

Due to the assumptions in the solution of Equation(2) for the case of constant diffusion coefficients, Equations(3)~(6) do not accurately represent practical drying behavior. However, these equations are still useful since they allow the easy estimation of diffusion coefficients from experimental results by minimizing the surface resistance.

2.3 Diffusion Coefficients

Equation(4) and Equation(6) are useful for determination of diffusion coefficients. Siau (1984) shows that Equation(4) is effective when Dt/a^2 is equal to or greater than 0.2, and the infinite series solution can be represented by the first term only. By solving the resulting equation in terms of D, Equation(4) becomes;

$$D = \frac{4a^2}{\pi^2 t}\left[\ln \frac{8}{\pi}\frac{(M-M_e)}{(M_i-M_e)}\right] \quad \cdots\cdots (7)$$

In Equation(6), the function ierfc(z) vanishes to zero when the value of z becomes large($z \geq 2$; Crank, 1975). Then the diffusion coefficient, D, can be calculated as follows;

$$D = \frac{\pi a^2}{4t}\left[\frac{(M-M_e)}{(M_i-M_e)}\right]^2 \quad \cdots\cdots (8)$$

Equation(7) and Equation(8) have been used to calculate the diffusion coefficient from drying experiments by many researchers.

As mentioned earlier, the solutions of Equation(2) are valid for the case of constant diffusion coefficient. Equation(7) and Equation(8), however, clearly show the dependence of the diffusion coefficient on the moisture concentration. This is true because the driving force for moisture diffusion was fundamentally assumed to be the moisture concentration gradient.

Dependence of the diffusion coefficient on moisture concentration can also be postulated by mathematical relationships for steady state and unsteady state conditions(Crank, 1975). For steady state conditions, the concentration dependent diffusion coefficient D_C can be deduced from a measurement of the flux, and represents a mean value over the range of concentration involved. By integrating the flux of steady flow over two concentrations, namely D_1 and D_2, diffusion coefficient D_C is given;

$$D_C = \frac{1}{C_1-C_2}\int_{C_2}^{C_1} D\,dC \quad \cdots\cdots (9)$$

Comstock(1963) and Choong(1965) measured the moisture dependence of diffusion coefficients D_C by a steady state method. Equation(9) was also extensively applied to unsteady state systems by Simpson(1974), and Simpson and Liu(1991).

Egner's method was applied by Skaar(1954), Stevens et al(1984), and Rice(1988) to measure the dependence of the diffusion coefficient on moisture concentration from unsteady state diffusion. This method requires two successive unsteady state moisture content gradients from which D_m can be determined by the relationship;

$$D_m = \left(\Delta \int_0^x MdX\right)\left(\frac{1}{\Delta t}\right)/\left(\frac{\Delta M}{\Delta x}\right) \quad \cdots\cdots (10)$$

The problem with this method is the tedious work required to determine the term($\Delta M/\Delta x$). A diffusion coefficient D_m calculated from this method is influenced by the localized variations of sorption properties of wood.

2.4 Boundary Conditions

The complication of using unsteady state diffusion in mathematical modeling arises from the continuously changing conditions at the surface of wood. In some cases, the surface boundary condition relates to the rate of transfer of the diffusing substance across the surface of the medium. The psychrometric consideration of mass transfer leads to the conclusion that the mass transfer of liquid from a solid by evaporation at the surface is exactly balanced by the heat supply from the ambient air. This may happen at the surface of wood during drying. and is considered as a surface boundary condition of Equation(2) as follows:

$$-D\left(\frac{\partial C}{\partial X}\right) = S(C_e - C_s) \quad \text{at } X = 0 \cdots\cdots \quad (11)$$

where S is a constant of proportionality or so called surface transfer coefficient. C_s and C_e are the actual concentration at the surface of wood at any time. and equilibrium concentration with the vapor pressure in the atmosphere remote from the surface. respectively.

Two more auxiliary conditions can be formulated from the symmetrical distribution of concentration along the center line of the width of a board and the uniform distribution of initial concentration through the thickness of a board as follows:

$$\left(\frac{\partial C}{\partial X}\right) = 0 \quad \text{at } X=0,\ C=C_i \ \text{ at } t=0 \cdots\cdots \quad (12)$$

3. NUMERICAL SOLUTION OF DIFFUSION EQUATION

A numerical approximation of Equation(2) can be computed by a finite difference method. An explicit forward method is computationally simple and widely used. One serious drawback of this method is that the process is valid only for $0 \leq r \leq 0.5$, where $r = \Delta t/(\Delta X)^2$, in which Δt and ΔX is an increment of time and distance. respectively: therefore the time step Δt should necessarily be small. The Crank-Nicolson implicit method is a method that reduces the total volume of computation, and is valid. ie. numerically stable and convergent. for all finite values of r.

For one-dimensional flow of moisture during drying into the radial direction from the tangential surface. Equation(2) can be partly non-dimensionalized by introducing new variables $x = X/a$ and $u = M/\rho$, where ρ is wood density. Now. x is a non-dimensional distance from 1 to -1 for the thickness of a board. and u is non-dimensional concentration. The resulting equation becomes.

$$\frac{\partial u}{\partial t} = \frac{D}{a^2}\frac{\partial^2 u}{\partial x^2} \cdots\cdots \quad (13)$$

with boundary conditions at the surface of a board and initial condition as:

$$\frac{\partial u}{\partial x} = \frac{L}{\rho}(u_e - u_s) \quad \text{at } x = \pm 1 \cdots\cdots \quad (14a)$$

$$u(x,\ 0) = u_i \quad \text{at } t = 0 \cdots\cdots \quad (14b)$$

where L is defined as Dt/a^2. Equation(13) with the initial condition and boundary conditions in Equation(14a) and(14b) can be approximated by the finite difference method. The Crank-Nicolson method replaces $\partial^2 u/\partial x^2$ by the mean of its finite difference representation on the$(j+1)$th and j th time row by:

$$\frac{u_{i,j+1} - u_{i,j}}{\Delta t} = \frac{D}{2a^2}\left[\frac{u_{i+1,j+1} - 2u_{i,j+1} + u_{i-1,j+1}}{\Delta x^2} + \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\Delta x^2}\right] \cdots\cdots (15)$$

where Δt and Δx are time and distance increments. respectively. By substituting $D\Delta t/a^2\Delta x^2$ as r and rearranging in terms of$(j+1)$th and$j$th row. Equation(15) can be written as:

$$-ru_{i-1,j+1} + (2+2r)u_{i,j+1} - ru_{i+1,j+1} = ru_{i-1,j} + (2-2r)u_{i,j} + r_{i+1,j} \cdots\cdots \quad (16)$$

In general, the left side of Equation(16) contains three unknown and the right side three known, pivotal values of u. Central difference representation of the boundary condition at the surface in Equation(14) for any time t at $x=\pm 1$, by imagination of the sheet extended one layer, is:

$$\frac{u_{1,j}-u_{-1,j}}{2\Delta x}=u_{0,j}-u_e \quad \cdots\cdots (17)$$

from which it follows that

$$u_{-1,j}=u_{1,j}-2h(u_{0,j}-u_e) \quad \cdots\cdots (18a)$$

$$u_{-1,j+1}=u_{1,j+1}-2h(u_{0,j+1}-u_e) \quad \cdots\cdots (18b)$$

where $h=(L/\rho)\Delta x$. By substituting Equation(18a) and(18b) into Equation(16) by inserting $i=0$ to eliminate $u_{-1,j}$ and $u_{-1,j+1}$. Equation (16) becomes:

$$-ru_{1,j+1}+(1+r+rh)u_{0,j+1}$$
$$=ru_{1,j}+(1-r-rh)u_{1,j}+2rhu_e \quad \cdots (19)$$

Using a similar method to determine the boundary condition to make use of the symmetrical moisture gradient at the center of the board, Equation(16) becomes another central difference equation as follows:

$$-ru_{N,j+1}+(1+r)u_{N-1,j+1}$$
$$=ru_{N,j}+(1-r)u_{N-1,j} \quad \cdots\cdots (20)$$

The explicit nature of the difference method in Equation(16) through(19) and(20) implies that this system can be written in the tridiagonal matrix form of equation as follows:

$$\begin{pmatrix} 1+r+h & -r & 0 & \cdots & 0 \\ -\frac{r}{2} & 1+r & -r & \cdots & 0 \\ 0 & -r & 1+r & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & -r & 1+r & -\frac{r}{2} \\ 0 & \cdots & \cdots & -r & 1+r \end{pmatrix} \begin{pmatrix} u_{1,j+1} \\ u_{2,j+1} \\ \vdots \\ \vdots \\ \vdots \\ u_{N-1,j+1} \end{pmatrix}$$

$$= \begin{pmatrix} 1-r-h & r & 0 & \cdots & 0 \\ \frac{r}{2} & 1-r & -r & \cdots & 0 \\ 0 & r & 1-r & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & r & 1-r & \frac{r}{2} \\ 0 & \cdots & \cdots & r & 1-r \end{pmatrix} \begin{pmatrix} u_{1,j} \\ u_{2,j} \\ \vdots \\ \vdots \\ \vdots \\ u_{N-1,j} \end{pmatrix} + \begin{pmatrix} rhu_e \\ 0 \\ \vdots \\ \vdots \\ \vdots \\ 0 \end{pmatrix} \quad \cdots\cdots (21)$$

With N internal mesh points along each time row then for $j=0$ and $i=1, 2,..., N$. Equation(21) gives N simultaneous equations for N unknown pivotal values along the first time row in terms of known initial and boundary values. Similarly, $j=1$ express N unknown values of u along the second time row in terms of the calculated values along the first, etc. A method such as this where the calculation of an unknown pivotal value necessitates the solution of a set of simultaneous equations is described as an implicit one.

The tensorial form of Equation(21) is $Au_{i,j+1}=Bu_{i,j}+C$, and the tridiagonal linear system of the equation can then be solved by LU decomposition method(Burden & Faires, 1993) where L and U are lower and upper diagonal matrixes of the matrix A and B. Verification of unconditionally stable convergent criteria using the Crank-Nicolson scheme on the order of $O(\Delta t^2+\Delta x^2)$ can be found in Isaacson and Keller(1966).

4. CONCLUSIONS

Under isothermal conditions of moisture transfer, drying behavior for the entire range of moisture content can be characterized by Fick's diffusion equation with convenient assumptions such as continuity of moisture profile and moisture dependent diffusion coefficient. Due to the complexity of exact solution of the governing equation, numerical analysis was preferred. Finite difference method was then employed to compute moisture profiles during drying of wood with suitable boundary conditions. Manipulation of mathematical works were accomplished with a FORTRAN program using a new algorithm of the Crank-Nicolson Scheme.

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