

Parameter estimation of moisture transfer in wood

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ABSTRACT: This study focuses on the bound water and liquid water transfer in wood and is to investigate moisture change and distribution of six wood species (three softwood and three hardwood) in the longitudinal direction exposed to the long term moisture sorption. This paper presents the results of experimental investigations of wood sorption in static environmental condition. Most of species used for the experiment arrived at estimated maximum moisture content and there might be no significant hysteresis in the capillary pressure curve due to air entrapment. The experimental data on the different samples were found to vary considerably. The Boltzmann transformation and Levenberg-Marquardt method were used to determine the liquid water diffusivity from measured moisture content profiles. For moisture content changes with time and moisture profiles, the validity was ascertained by comparing the numerical results with the corresponding experimental measurements. There was the abrupt change of the slope of the diffusivity function around fiber saturation point, which might seriously slow down the numerical solution process or even lead to a non-convergence condition.

Keywords: inverse method, wood, sorption, moisture transfer, parameter estimation, finite volume method

1. INTRODUCTION

Wood is a typical hygroscopic porous material and consists of cell wall, cavities and pits between cell walls. Moisture in wood exists as three phases of bound water, water vapor, and free(or liquid) water. Wood is susceptible for the growth bacteria, fungi, or algae, especially exposed high humidity conditions or to liquid water. Liquid water may provide a medium for diffusion of the enzymes or other metabolites by which biological deterioration can be expedited. The deterioration of decayed wood may be

accelerated by possible physical and chemical damages. The durability in wooden building largely depends on moisture condition. For wooden building of traditional post and beam structures, moisture content is kept below FSP during general use. However, columns may be exposed directly to the driving rain and can contact with liquid water. In addition, moisture may enter by condensation and run off from roof and facade, and capillary rising of ground water. Under certain environmental conditions, therefore, simulations of moisture transport process in

wood would be valuable for predicting susceptibility for the biological decay.

There is little work to measure and model moisture sorption in wood that moisture increases from low to high moisture content (Kumaran, 1999; Mukhopadhyaya, 2002; Virta et al., 2006).

Descamps (1996) reported that the optimization method with spline function performs better than Boltzmann transformation method and moisture gradient method because it does not use derivative of a moisture profile. However, the optimization methods have some serious limitations and different initial settings can lead to different optimization results. Sometimes the functions become over-parameterised and the same curve can be generated by different parameter combinations. It is also helpful to use expressions with parameters that can be directly obtained from the experiments. The goodness of the fit depends on a good guess of initial parameters.

The purpose of this paper is to investigate moisture change and distribution of six wood species (three softwood and three hardwood) in the longitudinal direction exposed to long term moisture sorption. Based on a transport model sorption, conductivities of bound water and free water covering the whole moisture range needed in the simulation of wood is determined by using the inverse method. In this study, the initial settings obtained by Boltzmann transformation method will be used and compared the accuracy. The validity is ascertained by comparing the numerical results with the corresponding experimental measurements.

2. THEORY

2.1 Moisture transfer model

Multiphase heat and mass transfer models that consider moisture content, air, and energy conservations were developed by several researchers (Moyne *et al.*, 1987; Turner, 1991; Perre *et al.* 1993; Couture *et al.*, 1995). If the gas pressure in wood is assumed to be constant, the mass transfer model can be converted to the diffusion equation.

$$\frac{\partial m}{\partial t} = \nabla \cdot \left[(D_w + \overline{D_v + D_B}) \nabla m \right] \quad (1)$$

where m :moisture content based on dry weight of wood(kg/kg), D_w : liquid water diffusivity(m^2/s), D_v : water vapor diffusivity(m^2/s), D_B : bound water diffusivity (m^2/s)

The liquid water diffusivity over hygroscopic range can be expressed by using the generalized Darcy's law.

$$D_w = -\frac{\rho_w}{\rho_0} \frac{k_{rw} K_w}{\mu_w} \frac{\partial P_c}{\partial S} \frac{\partial S}{\partial m} \quad \forall m > m_{FSP} \quad (2)$$

where k_{rw} : relative water permeability(-), K_w : intrinsic water permeability(m^2), μ_w :dynamic viscosity of liquid water(Pa s), P_c : capillary pressure(Pa), ρ_0 : dry wood density(kg/m^3), ρ_w : liquid water density (kg/m^3), k_{rw} : relative water permeability(-), K_w : intrinsic water permeability(m^2), μ_w :dynamic viscosity of liquid water(Pa s), P_c : capillary pressure(Pa), S : liquid water saturation(-), D_v : diffusivity of water vapor (m^2/s), D_b :diffusivity of bound water(m^2/s).

The combined diffusion coefficient under the isothermal condition is expressed into different equations depending on models (Kang et al., 2008).

$$\begin{aligned} \overline{D_v + D_B} = D_{bc} = & p\sqrt{\phi}D_v \\ & + \frac{\sqrt{\phi}(\sqrt{\phi} - p)(L + 1 - \sqrt{\phi})\rho_c^m D_{BL}}{1 - \sqrt{\phi} + L\rho_c^m D_{BL} / D_v} + (1 - \phi)\rho_c^m D_{BL} \end{aligned} \quad (3)$$

where p :the ratio of an effective pit opening area to end wall area; L :the ratio of fiber length to an effective diameter, D_v : diffusivity of water vapor in air(m^2/s), D_{BL} : longitudinal diffusivity of bound water in the cell wall, ϕ : porosity or void fraction(-)

The porosity of wood may be calculated from wood and cell wall density using Eq. (4), assuming that the density of bound water is equal to the water density, the oven-dry cell wall density is $1530\text{kg}/\text{m}^3$, and the pore volume remains constant with the moisture changes (Siau, 1995).

$$\phi = 1 - \frac{\rho^m}{\rho_c^m} = 1 - \frac{\rho_o}{1 + m\rho_o/1000} \frac{1 + 1.53m}{1530} \quad \forall m \leq m_{fsp} \quad (4)$$

where ρ_c^m and ρ_o^m : wood and cell wall density based on oven dry weight and moist volume (1530 kg/m³)

Bound water diffusion coefficient in the longitudinal direction can be estimated from transverse one,

$$D_{BT} = 7 \times 10^{-6} \exp[-(38500 - 29000m) / RT] \quad (5)$$

$$D_{BL} = 2.5 \times D_{BT} \quad (6)$$

and water vapor diffusion coefficient is

$$D_v = D_{av} \frac{0.018 p_{vs}}{\rho_c^m RT} \frac{\partial h}{\partial m} \quad (7)$$

$$D_{av} = 2.2 \times 10^{-5} \left(\frac{1.013 \cdot 10^5}{P} \right) \cdot \left(\frac{T}{273} \right)^{1.75} \quad (8)$$

where R : universal gas constant (8.314 J/mol K), T : Kelvin temperature (K), p_{vs} : saturated vapor pressure (Pa), h : relative humidity, P : total pressure of air and water vapor (Pa)

According to Siau(1995), the Eq.(3) may be expressed into simplified one.

$$D_{bc} = \frac{\phi}{1 - \phi} \frac{D_v D_{BL}}{D_{BL} + (1 - \sqrt{\phi}) D_v / L} \quad (9)$$

The maximum possible moisture content of wood is predicted theoretically if the cell cavities remain constant in size during the moisture sorption and M_{FSP} is known.

$$m_{max} = m_{FSP} + \frac{\phi}{G_0} \quad (10)$$

where the fiber saturation point of wood m_{FSP} is usually assumed to be 0.3 and G_0 is the dry specific gravity of wood.

However, it is difficult to measure the dry volume because the moisture content can be changed during measuring. Therefore, the dry specific gravity can be obtained using the moist one.

$$G_0 = \frac{G_m}{1 - m G_m} \quad (11)$$

where G_m is the specific gravity of wood based on dry weight and moist volume at moisture content m .

2.2 Numerical analysis

The governing equation to isothermal moisture transfer can be obtained by substituting Eq. (3) into Eq. (1).

$$\begin{aligned} \frac{\partial m}{\partial t} &= \nabla \cdot [(D_w + D_{bc}) \nabla m] \\ &= \nabla \cdot [D \nabla m] \end{aligned} \quad (12)$$

2.2.1 Finite volume method

Consider the non-linear diffusion equation

$$\frac{\partial m}{\partial t} = \frac{\partial}{\partial x} \left[D(m) \frac{\partial m}{\partial x} \right] \quad t > 0, \quad 0 \leq x \leq L \quad (13)$$

with some initial condition

$$m(x, 0) = m_0(x), \quad 0 \leq x \leq L \quad (14)$$

and two points boundary conditions

$$\begin{aligned} D \frac{\partial m}{\partial x} &= h[m(L, t) - 0.05] \quad \text{at } x(L, t) \\ m(0, t) &= m_{max} \end{aligned} \quad (15)$$

where h is the external convective mass transfer coefficient ($h=0.0001/\rho_0$).

In order to find the solution of Eq. (13) by the finite volume method, we take some mesh

$$\Pi = \{(x_i, t_j) | 0 = t_0 < t_1 < \dots < t_n, \quad 0 = x_0 < x_1 < \dots < x_m = L\} \quad (16)$$

and construct an appropriate control volume corresponding spatial nodes $\{x_i\}$. By integrating Eq. (13) on each control volume(Figure 1) and using the Gauss-divergence theorem, we have following discrete form

$$\frac{m_i^{j+1} - m_i^j}{\Delta t^j} = \sum_{f=E,W} [D(m^{j+1}) \frac{\partial m^{j+1}}{\partial x} \cdot n]_f \quad (17)$$

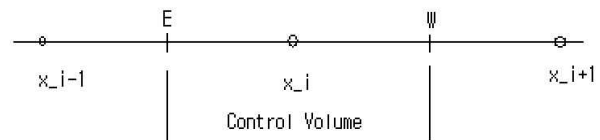


Figure 1. Nodes and control volume

where superscript (j) means time layer and subscript (i) means nodes and n_f means outward normal vector at each end points of the control volume. At the end points

W , the value of the $D(m^{j+1})$ is given by average value

$$D(m^{j+1})|_W = (D(m_i^{j+1}) + D(m_{i+1}^{j+1})) / 2 \quad (18)$$

and the derivative is approximated by numerically

$$\frac{\partial m^{j+1}}{\partial x} = \frac{m_{i+1}^{j+1} - m_i^{j+1}}{x_{i+1} - x_i} \quad (19)$$

At the $(j+1)$ -th time, we know the solution $m^{(j)}$ at the (j) -th time. Hence, as shown in Eq. (19), each equation can be obtained m_{i-1}^{j+1} , m_i^{j+1} , and m_{i+1}^{j+1} . However, the system of equations must be non-linear. So that we use the iterative method, such as the Newton's iteration.

2.2.2 Diffusivity

For adopting the generalized Darcy's Law to the simulation, it requires the intrinsic and relative permeability as well as capillary-liquid water relation. For the combined diffusion coefficient to, it requires the information of cell wall geometry as well as sorption isotherm. There are no sufficient data on them until now. Therefore, two types of diffusion coefficient are assumed as follows.

First, one coefficient is proposed by the exponential function with the third-degree polynomials, which is continuous in the whole moisture content range.

$$D = \exp(a_0 + a_1 m + a_2 m^2 + a_3 m^3) \quad (20)$$

Second, two coefficients are proposed by the exponential function. They have the third-degree polynomials over the hygroscopic range and the first order in the hygroscopic range.

$$\begin{aligned} D_w &= \exp(a_0 + a_1 m + a_2 m^2 + a_3 m^3) \\ &\quad \forall m > m_{FSP} \\ D_{bc} &= \exp(a_0 + a_1 m) \quad \forall m \leq m_{FSP} \end{aligned} \quad (21)$$

2.2.3 Levenberg-Marquardt method and Gauss-Newton Method

Suppose that we don't know and must determine the value of the coefficient $D(m)$ by using the experimental result m_i^j 's for some i and j . Since we have the 4

parameters a_0, a_1, a_2 and a_3 , but many experimental data m_i^j 's are given. In this case we commonly use the least-square method as follows:

To find the parameters $A = [a_0, a_1, a_2, a_3]$ that minimize the objective functional, it was defined as the sum of the squares of the deviation between the measured and the predicted data on both average moisture content and a moisture profile.

$$\begin{aligned} F(A) &= \sum_{j=1}^N [\bar{m}(t_j) - \bar{m}_e(t_j)]^2 \\ &\quad + \sum_{k=1}^M [m(x_k, t_N) - m_e(x_k, t_N)]^2 \end{aligned} \quad (22)$$

$\bar{m}$ and $\bar{m}_e$ is average moisture content of predicted and experimental data with time t , respectively. $m_e(x_k, t_N)$ is moisture profile of the experimental data for final time t_N and $m(x_k, t_N)$ is one of numerical solution for the nonlinear diffusion equation (13) by finite volume method explained at section 2.2.1.

The necessary conditions that the functional is minimized at the A^* is

$$\nabla F(A^*) = 0 \quad (23)$$

Then the gradient of $F(A)$ is

$$\nabla F(A) = \sum_{i=1}^m r_j(A) \nabla r_i(A) = J(A)^T r(A) \quad (24)$$

where $r(A) = (r_1, r_2, \dots, r_m)^T$,

$$r_i(A) = \bar{m}(t^i) - \bar{m}_e(t^i) \quad i = 1 \dots N$$

$$\begin{aligned} r_{N+k}(A) &= m(x_k, t^N) - m_e(x_k, t^N) \quad k = 1 \dots M \\ m &= N + M \end{aligned}$$

And the Jacobian matrix of $r(A)$ is

$$J(A) = \begin{pmatrix} \frac{\partial r_1}{\partial a_0} & \frac{\partial r_1}{\partial a_1} & \frac{\partial r_1}{\partial a_2} & \frac{\partial r_1}{\partial a_3} \\ \frac{\partial r_2}{\partial a_0} & \frac{\partial r_2}{\partial a_1} & \frac{\partial r_2}{\partial a_2} & \frac{\partial r_2}{\partial a_3} \\ \vdots & \vdots & \vdots & \vdots \\ \frac{\partial r_m}{\partial a_0} & \frac{\partial r_m}{\partial a_1} & \frac{\partial r_m}{\partial a_2} & \frac{\partial r_m}{\partial a_3} \end{pmatrix} \quad (25)$$

But this system of the equations is difficult to compute and nonlinear. Hence the Newton's method is used to solve this

system. The original Newton's iterative formula has the form.

$$A^{(k+1)} = A^{(k)} - [J(A^{(k)})^T J(A^{(k)}) + S(A^{(k)})]^{-1} J(A^{(k)})^T r(A^{(k)}) \quad (26)$$

where Hessian $S(A)$ has the second-order derivative such as

$$S(A) = \sum_{i=1} r_i(x) \nabla^2 r_i(x) \quad (27)$$

However, $S(A)$ is expensive to compute and make the system ill-conditioned. Hence, by neglecting this second-order term in Newton's method, the simplified iteration is following:

$$A^{(k+1)} = A^{(k)} - [J(A^{(k)})^T J(A^{(k)})]^{-1} J(A^{(k)})^T r(A^{(k)}) \quad (28)$$

This equation is said to be the Gauss-Newton iteration. To make the iteration well-defined, it is required that the rank of the Jacobian matrix is 4. Obviously, the success of Gauss-Newton method will depend on the importance of the neglected second-order term $S(A)$. If $S(A^*) = 0$, the Gauss-Newton method would have quadratic convergence rate.

3. MATERIALS AND METHODS

Each three of softwood and hardwood were selected for the experiments (Table 1). Wood samples were cut with a prismatic shape of approximate dimensions $w \times d \times h = 25 \times 25 \times 200 \text{ mm}^3$. The four vertical sides were coated by varnish with heavy pigments. The top and bottom were left unpainted.

The bottom surface was submerged only a few millimeters in order to avoid build-up of hydrostatic pressure. The top surface was exposed to ambient condition. The environmental laboratory conditions were kept constant at 20°C and 40 % RH during the experiments.

For all the samples, their moistures were recorded at various time intervals. The moisture of each sample in grams was obtained by subtracting the moisture of the oven dried samples from the moisture of the moist samples. After the sorption test, the specimen was cut

consecutively into 24 to 27 pieces for measuring moisture and specific gravity distributions. The volume for the specific gravity was measured by water immersion method after both uncoated surfaces were coated with paraffin.

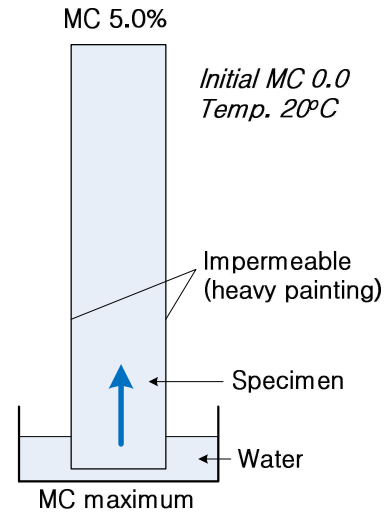


Figure 2. Schematic diagram of the moisture sorption test.

4. RESULTS AND DISCUSSION

4.1 Maximum Moisture Content

The estimation of maximum moisture content is important for predicting the sorption process of wood accurately, which should be defined at the boundary conditions. Using Eq. (4), most of estimated maximum MC was slightly higher than measured one, as expected. The difference between estimated and measured maximum moisture content might be due to lower FSP, air entrapment, dead pore. The difference in hardwood was higher than softwood. However, Eq. (3) would be used to estimate the maximum moisture content theoretically.

4.2 Estimation of Moisture Diffusivity

Moisture content changes with time and moisture distributions at the final stage were shown in Figure 3. The moisture diffusivity was obtained by Boltzmann transformation method over the whole moisture content (Table 2 and 3). The shape of the curve representing the dependence of diffusion coefficients with moisture content was similar in all wood, and the diffusivity decreased with moisture content until FSP

and then increased. Adopting them to moisture transfer equation(Eq. (12)), the simulation results gave poor predictions for moisture content changes with time and moisture distributions because Boltzmann transformation method is valid for a semi-infinite volume and a linear correlation between moisture flux and square root of time.

Mathematically, the inverse problems belong to the class of ill-posed problems. The solution does not satisfy the general requirements of existence, uniqueness, and stability under small changes to the input data(Ozisik, 1993). The inverse solutions are known to be very sensitive to small changes in input data resulting from measurement and modeling errors. Therefore the initial input values of parameters obtained by Boltzmann transformation method were used as a first approximation for Levenberg-Marquardt method, which resulted in much better prediction for moisture change and moisture prediction(Figure 3).

Both experimental and model-based determination of phase-separated transport properties is still one of the most disputed issues in moisture transport analysis. However, this study shows that there is distinctive hygroscopic zone in wood. For sorption simulation, diffusivity should be separated into hygroscopic and non-hygroscopic zones.

5. CONCLUSION

For sorption test, the experimental data on the different samples were found to vary considerably. The result of single side water soaking shows that density is the main factor that influences the absorption properties. Levenberg-Marquardt method can be used to determine the liquid water and combined bound water diffusivity from measured moisture content profiles. The initial input values of parameters by the Boltzmann transformation method were used as a first approximation for Levenberg-Marquardt method. For moisture content changes with time and moisture profiles, the validity was ascertained by comparing the numerical results with the corresponding experimental measurements. There was the abrupt change of the slope of the diffusivity

function around fiber saturation point, which might seriously slow down the numerical solution process or even lead to a non-convergence condition. The results of this study would be useful in the process of sorption for exterior wood and dipping for preservation treatments,

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Table 1. Physical properties of wood species used for the experiment

Species		Duration (month)	Dry density (kg/m ³)	Porosity	Maximum MC (kg/kg)		Δ MC ¹⁾
					Estimated	Measured	
Softwood	Hemlock (<i>Tsuga heterophylla</i>)	1	442	0.71	1.92	1.80	0.12
		2	421	0.72	2.03	2.02	0.01
	Radiata pine (<i>Pinus radiata</i>)	1	412	0.73	2.08	1.94	0.14
		2	480	0.69	1.74	1.74	0.00
	Spruce (<i>Picea mariana</i>)	1	509	0.67	1.61	1.61	0.00
		2	481	0.69	1.73	1.69	0.04
Hardwood	Painted maple (<i>Acer mono</i>)	1	620	0.59	1.26	1.21	0.05
		2	629	0.59	1.24	1.03	0.11
	Japanese elm (<i>Ulmus davidiana</i>)	1	783	0.49	0.93	0.86	0.07
		2	637	0.58	1.22	1.03	0.09
	Horn beam (<i>Carpinus cordata</i>)	1	722	0.53	1.04	0.90	0.14
		2	713	0.53	1.05	0.93	0.12

¹⁾ Differential moisture content between estimated and measured maximum moisture content

Table 2. Diffusion coefficients with the continuous function by the inverse method, Eq. (20)

Species		Duration (month)	a_0	a_1	a_2	a_3	F	
							LM ¹⁾	BT ²⁾
Softwood	Hemlock	1	-22.35	3.571	-7.875	3.849	0.161	0.777
		2	-22.37	1.880	-4.050	1.969	0.102	0.160
	Radiata pine	1	-21.05	-5.596	8.226	-2.714	0.524	0.608
		2	-21.52	-6.264	8.237	-2.276	0.575	3.001
	Spruce	1	-21.80	-4.354	8.995	-3.552	0.266	0.377
		2	-21.49	-6.456	8.889	-2.592	0.408	0.438
Hardwood	Painted maple	1	-16.35	-17.63	24.09	-8.392	0.140	15.53
		2	-18.14	-14.84	28.25	-13.37	0.125	7.092
	Japanese elm	1	-21.01	-4.527	7.630	0.381	0.146	0.146
		2	-21.62	-0.857	-6.190	8.955	0.361	0.469
	Horn beam	1	-21.52	-3.563	-1.538	9.700	0.046	0.246
		2	-21.45	-6.995	20.57	-12.78	0.016	0.020

Table 3. Diffusion coefficients with two step functions by the inverse method, Eq. (21)

Species		Duration (month)	a_0	a_1	a_2	a_3	b_0	b_1	F	
									LM ¹⁾	BT ²⁾
Softwood	Hemlock	1	-24.83	9.567	-11.99	4.706	17.95	14.87	0.042	0.320
		2	-22.58	2.552	-5.179	2.407	19.95	10.35	0.056	10.22
	Radiata pine	1	-20.32	-14.49	18.70	-5.887	18.64	12.66	0.272	2.055
		2	-21.59	-2.453	1.298	0.610	19.65	3.574	0.333	4.873
	Spruce	1	-23.76	4.817	-1.515	-0.014	17.68	9.609	0.118	0.192
		2	-20.27	-11.93	14.85	-4.384	15.96	21.40	0.059	0.664
Hardwood	Painted maple	1	-19.55	-10.29	18.67	-7.152	17.72	9.629	0.114	1.475
		2	-25.12	16.79	-19.86	10.34	18.87	3.010	0.078	8.431
	Japanese elm	1	-24.09	17.41	-32.35	22.32	13.74	34.61	0.064	0.115
		2	-23.18	14.72	-33.27	22.41	15.69	19.33	0.078	0.901
	Horn beam	1	-29.98	44.12	-82.70	52.86	19.26	11.15	0.028	0.153
		2	-22.93	2.491	3.353	-3.284	19.37	10.86	0.037	0.330

¹⁾Levenberg-Marquardt Method, ²⁾Boltzmann transformation method

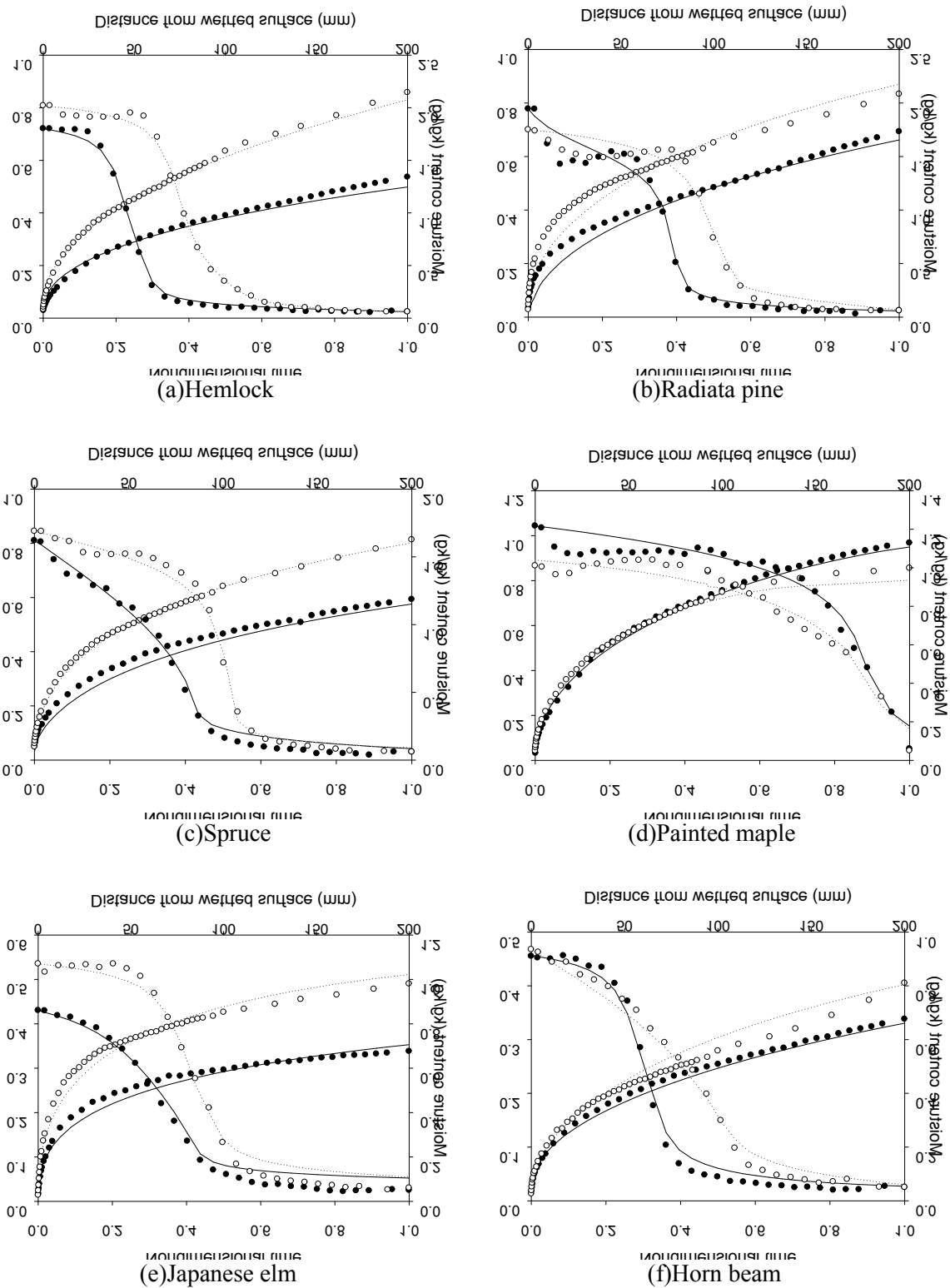


Figure 3. Comparison of measured and predicted average moisture content change and moisture distribution using two steps of moisture diffusion coefficient by the Levenberg-Marquardt inverse method. Measured : ● 1month, ○ 2month. Predicted : solid line-1 month, dotted line-2 month.