

## Inverse Method Using TransPore 1-D Code for The Mass-Diffusivity Determination In Wood

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### ABSTRACT

In this study, the diffusion coefficient of bound water in wood was estimated using three steps: an original experiment, a TransPore-based simulation and an inverse method of identifying the value of the desired physical quantity. The excellent agreement between the calculated weight and the measured weight gives an idea of the effectiveness of this method. The main advantage of this method lies in the rigorous analysis of the experimental data. Indeed, this rigor is characterized by taking into account the coupling between thermal and mass transfer and especially the real climate conditions experienced by the samples. All these qualities give these method major advantages: reliability, speed and routine measurement. This is not the case of old classical and numerical methods.

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### Introduction

The mass-diffusivity in the hygroscopic field of the wood is one of the transfer properties which characterize the migration of the bound moisture. Although being physical parameters in which the scientists are interested for decades, the mass-diffusivity remains regrettable, nowadays, always handicapped by difficulties inherent in its determination. The research for reliable and fast technical leads the scientists to propose various approaches so theoretical as experimental.

Under steady-state conditions, the determination of the mass diffusivity consists in measuring, up to equilibrium, the evolution of the mass of a sample of wood subjected on both sides to two different moisture relative humidity. The technique involves covering a glass with a sample of wood. Inside the glass, there is usually a saturated solution of salt that regulates the relative humidity. The glass is then placed on a weighing scale in climatic chamber with controlled relative humidity. The relative humidity gradient thus created on either side of the sample will cause moisture transfer in the wood sample. The weighing scale makes it possible to measure the evolution of the mass of the sample over time. In this field, the work of [1] remains one of the originality because it had the merit to take into account the peculiarity of the wood with the installation of a system composed of PVC and inner tube which favors the diffusion of moisture only according to the thickness of the sample. his tests lasted more than 10 days per sample.

Most of methods of the mass-diffusivity measurements proposed presently in transient regime are generally based on the successive weighing technique [2-3]. The implementation of this technique is very demanding from the experimental point of view. But the possibility of using numerical tool, in an inverse method, can help to reduce these experimental requirements.

The inverse method is an indirect technique of parameters determination. Its use needs a perfect experimentation and

a very faithful physical model to the experimental configuration. This method consists of three stages: testing, physical model and minimization of the difference between experiment and model.

In literature, several works have been done on the use of inverse method in numerous physical sectors. In thermal science for example, we can cited those of [4-9]. We can also quoted those of [10-14] on the determination of the mass-diffusivity in wood. For many of these studies on mass-diffusivity, the numerical resolutions of mass-transfer equations was done generally with such simplifications like in case of simple analytical resolutions. So, if the coupled between heat and mass transfer (condensation on the sample or evaporation from the sample) is not neglected, it's rather the external resistance of transfer [14-15]. In such context, mass-diffusivity was determined with a big mistake.

The aim of this study is to use, in an inverse approach, a numerical model noted TransPore1-D [16] for the determination of the mass-diffusivity in the wood. This numerical code is complete and taken into account the coupling between heat and mass in this type of transfer [17-19]. Indeed, the macroscopic equations about internal heat and mass transfers in a wood sample and relevant initial and boundary were numerically solved. This leads to predict the profile of moisture average and temperatures in the sample at specified moments. The mass of sample can then be calculated as function of time. A sorption experimental device used in previous studies at LERMAB Laboratory (Laboratoire d'Etude et de Recherche sur le Matériau Bois) at Nancy in France has been improved to collect the sample mass and the climatic conditions undergo by the sample. The theoretical values of sample mass are compared with experimental values by using the criterion of least squares. The optimization method of Simplex allows us to find out the mass-diffusivity which minimizes the deviation between the simulated and measured mass of the sample. In addition to mass-

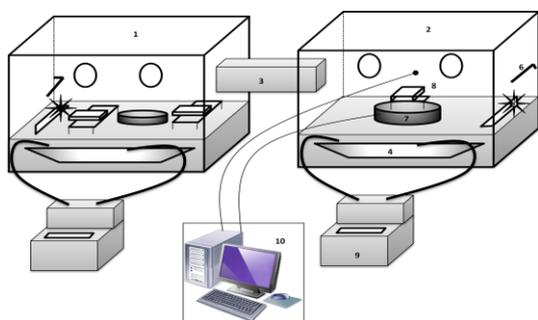
diffusivity determination, three unknown parameters are estimated for the accuracy of the method. Sensitivity analysis has allowed us to determine the sensitivity of each estimated parameters on the theoretical mass simulated and to know if all parameters can be estimated simultaneously. The validity of this method is shown by the agreement between the result of the duplicate samples and weakness of the global relative error.

## Experimental

### Experimental setup

Experiment is based on the monitoring of the mass and environmental conditions of the wood sample in the climatic chamber. These parameters are measured in real-time. An adapted device for transient measure of mass-diffusivity is used (Fig.1). This device was also used by [14] and [15] for their previous work on mass diffusion in wood. In overall, it consists of:

- two identical climatic chamber (chamber 1 and 2). Each climatic chamber is set at a dry bulb temperature equal to 35°C. The relative humidity of the air in the chamber is controlled by water bath maintained at constant temperature via a Cryothermostat. The temperature of the water has just been set at the desired dew point temperature. A ventilator helps to harmonize the relative humidity in each chamber. Both chambers are connected with a sealed airlock. This airlock allows to move samples from one chamber to another.
- two electronics balances accurate at 0,001g. Each chamber has a balance. One is used to measure continuously the mass of the sample and the other to check its hygroscopic equilibrium. To avoid the air flow disturbance into the chamber, the balance is equipped with a glass frame from which all sides are closed but its higher face is opened to allow the sample to be in contact with the chamber ambiance.
- a relative humidity sensor and platinum resistance thermometer (Pt100) were placed in the vicinity of the exchange surface of the samples. These are measured and recorded the actual environmental conditions undergone by the samples. The sensor is connected to the data acquisition device (Hewlett-Packard HP 34970A). The latter and the electronic balance are connected directly to the computer via RS-232 connections. The two units of measurements are controlled by software developed in *Visual Basic* and *Turbo Pascal*.



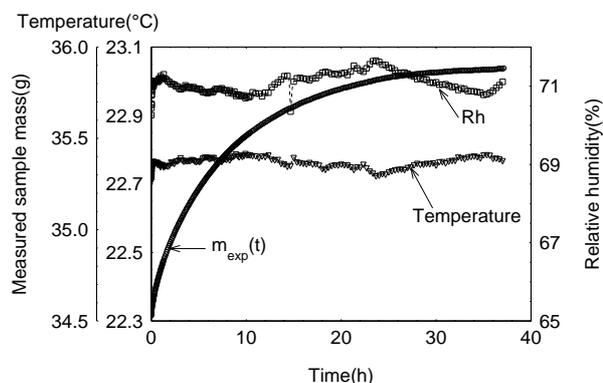
**Figure 1:** Experimental setup : (1) saturated climatic chamber, (2) sorption climatic chamber, (3) sealed airlock, (4) water bath, (5) ventilator, (6) PID temperature controller, (7) electronics balances, (8) wood sample on the balance, (9) Cryothermostat, (10) computer

### Sample preparation and sorption experiment

The sample preparation does not require substantial resources. Surely enough, the samples were a simple parallelepiped. Their dimensions are 100×50×5mm<sup>3</sup>. They are cut along wood material direction. The sample thickness is along the radial (R) or the tangential (T) direction, depending on characterized direction. The sample laterals sides are sealed with a thin layer of epoxy resin in order to limit the bound moisture spread at the thickness. We can use not only parallelepiped samples but also cylindrical Samples. Tests were made in absorption on three species: violet wood (*peltogyne spp.*), ipe (*tabebuia spp.*), and European beech (*Fagus sylvatica L.*). For radial and tangential thickness of each species, two samples were cut side by side in order to have matched samples.

All samples were saturated in the first climatic chamber at about 30% of relative humidity (Rh) and 35°C of temperature (T). After that, they were moved, one by one, to the second climatic chamber at about 70% relative humidity and 35°C of temperature. Indeed, each day, a saturated sample is putted on the balance in the second climatic chamber where the mass and environmental data are collected continuously. Even if the sample stabilization is not reached in this chamber, the stored data are enough for the mass-diffusivity extraction by inverse method developed in this study. This allows us to gain on the experimental duration.

An example of measurements on a European beech (*Fagus sylvatica L.*) sample is illustrated in Fig.2. The evolution of the sample mass shows well enough the absorption of water vapour by the sample. The regularity of the relative humidity values shows that the climatic chamber is well airtight. However, any incident or unexpected change of the climatic chamber condition is automatically taken into account in the numerical *TransPore* code because the latter are used as input data.



**Figure 2:** an experimental data example

### Theoretical calculation of sample mass

The theoretical calculation requires the moisture content field within the sample to be known at any time. For this reason, the *TransPore* code is used. This code solves a very comprehensive set of macroscopic equations to describe the coupling between heat and mass transfer in porous media. Several version of this code do exist: 1-D to 3-D for structured or unstructured meshes [16, 20]. The important details of the drying transport equations are summarised in these articles. Because the sample thickness is less than the other dimensions, the very fast 1-D version of *TransPore* is the most appropriate option.

According to the experiment and the sample configuration , its mass  $m_{th}(t)$  was determined by:

$$m_{th}(t) = m_{dry} \times [\bar{X}(t) + 1] + m_{res} \quad (1)$$

Where  $m_{dry}$  is the dry mass of the sample;  $\bar{X}(t)$ , the sample average moisture content; and  $m_{res}$ , the mass of epoxy resin used to seal the lateral face of sample. For the simulation, Eq.1 was fitted into *TransPore 1-D*. Consequently, using only to experimental data, namely temperature, relative humidity and external heat and mass transfer coefficients, this computational model is able to simulate the time evolution of internal pressure, temperature and moisture field evolution within the board, and then the time evolution of theoretical sample mass  $m_{th}$ . Figure 3 shows an example of calculated mass with a specific and measured input data. Rh and T are the measured relative humidity and temperature in the climatic chamber.

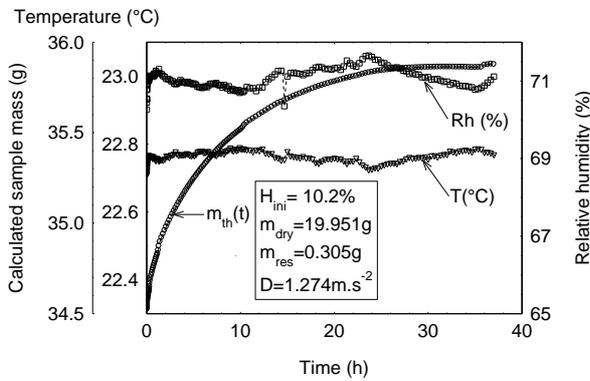


Figure 3 : Calculated sample mass  $m_{th}(t)$  with relevant parameters and real experimental input data

**Sensitivity analysis**

Since  $m_{th}(t)$  was predicted by *TransPore*, its value was largely depended on unknown sensitive *TransPore* parameters, namely mass-diffusivity (D) and initial bound moisture ( $X_{ini}$ ). At all,  $m_{th}(t)$  is depended on four parameters:  $D, X_{ini}, m_{dry}$  and  $m_{res}$ .

In order to justify the prediction of the parameters, relative sensitivities of the theoretical mass  $m_{th}$  to  $m_{dry}, m_{res}, X_{ini}$  and D parameters were determined respectively by:

$$S_{m_{dry}} = m_{dry} \cdot \frac{\partial m_{th}}{\partial m_{dry}}; S_{m_{res}} = m_{res} \cdot \frac{\partial m_{th}}{\partial m_{res}}; S_{X_{ini}} = X_{ini} \cdot \frac{\partial m_{th}}{\partial X_{ini}} \text{ and } S_D = D \cdot \frac{\partial m_{th}}{\partial D} \quad (2)$$

Because  $m_{th}$  is not explicitly function of these parameters, numerical derivation can be used. According to [7], partial numerical derivation of  $m_{th}$  over D can be calculated by:

$$\frac{\partial m_{th}(m_{dry}, m_{res}, X_{ini}, D)}{\partial D} = \frac{m_{th}(m_{dry}, m_{res}, X_{ini}, D + \delta D) - m_{th}(m_{dry}, m_{res}, X_{ini}, D)}{\delta D} \quad (3)$$

Where  $m_{th}(m_{dry}, m_{res}, X_{ini}, D)$  is the predict value of theoretical mass at the optimal value of  $m_{dry}, m_{res}, X_{ini}$ , and D. The same calculation will be done for the others parameters.

For this study, relative sensitivities were calculated with 1% disturbance of parameters. This corresponds to:

$$\delta D = 0.01D; \delta m_{dry} = 0.01m_{dry}; \delta m_{res} = 0.01m_{res}; \delta X_{ini} = 0.01X_{ini} \quad (4)$$

Relative sensitivities curves are plotted on Fig. 4. It can be seen that the theoretical mass is sensitive to both parameters. Principally, its sensitivity to D ( $S_D$ ) is good and attains its maximum at 10 hours.

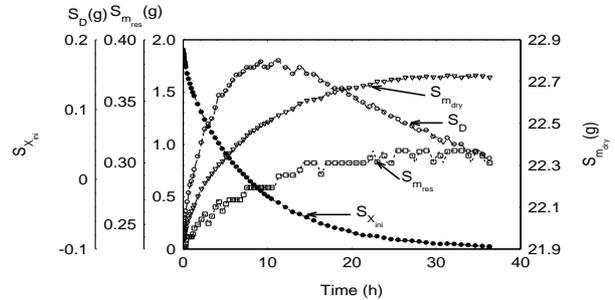


Figure 4 : Relative sensitivities curves to D, Xini, mdry and mres

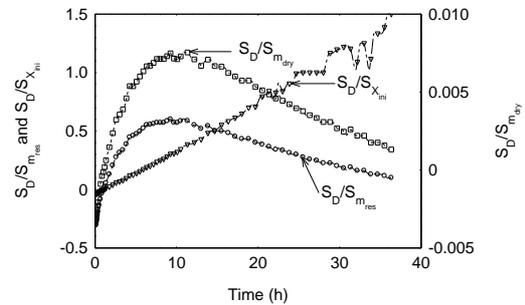


Figure 5 : Relation between sensitivity to D and sensitivities to others parameters

In Fig. 5, the ratio  $S_D/S_{m_{res}}, S_D/S_{m_{dry}}$  and  $S_D/S_{X_{ini}}$  are plotted as a function of time. This shows that the curves are not constant or the sensitivities are linearly independent (otherwise the curve would be part of a line parallel to x-axis). Consequently both parameters can be estimated at the same time. The choice of these parameters is guided by the fact that they are not well known ( $X_{ini}$ ) or unknown ( $m_{res}, m_{dry}$  and D). From this list, only the diffusion coefficient, D, is the interesting result for us.

**Parameters identification**

The third phase of the mass diffusivity determination by inverse method is the definition and minimization of the  $\delta$  objective function. This expresses the deviation between the measured and predicted mass. It was defined as the square sum of difference between the predicted and measured value of the sample mass (eq.5). It also, as  $m_{th}$ , depends on D,  $X_{ini}, m_{dry}$  and  $m_{res}$ .

$$\delta(D, X_{ini}, m_{dry}, m_{res}) = \frac{1}{k} \times \sqrt{\sum_{j=1}^k [m_{th}(j) - m_{exp}(j)]^2} \quad (5)$$

Where  $m_{exp}(j)$  is the  $j^{th}$  mass measured by the electronic balance,  $m_{th}(j)$  is the  $j^{th}$  mass predicted by the code *TransPore*, D is the mass diffusivity and  $X_{ini}$  is the initial moisture content of the sample (saturated moisture content).

The minimization of this objective function reduces the gap between experimental and theoretical curves of the mass by the adjustment of sensitive parameters. Several

methods of minimization have been developed in literature. They are applied to the function of one or more variables. Among them: minimization by successive frames, by gradient descent, by conjugate gradient, and so on. These methods can be found in the book named « Numerical Recipes » [21].

In this study, the algorithm "Simplex" called "Downhill simplex method" due to [22], which applies to the function of several variables, is most suitable. Indeed, contrary to other algorithms, any derivation of function is necessary.

This Simplex algorithm is used to evaluate the optimal values of the variables that minimize the objective function. Thus, each calculation of  $\delta$  requires a complete simulation of the experience with *TransPore* for a set of parameters  $m_{dry}$ ,  $m_{res}$ ,  $X_{ini}$  and  $D$ . The simulations will continue until the minimum value of  $\delta$  is reached. At this minimum, the values of  $D$  and other parameters are identified. However, the risk of identifying local minima is great. The choice of effective input parameters and the check of the agreement between the measured and identified curves at the minimum of the objective function allow to have reliable results. In all, the identification procedure took less than one minute per sample.

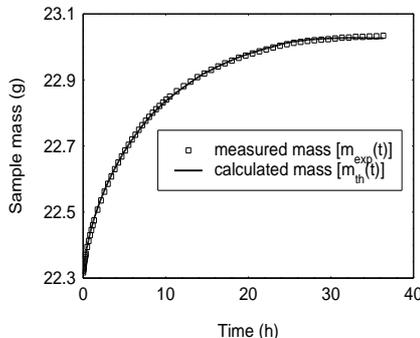
At the minimum of the objective function, we have defined the global relative error  $e_g(\%)$ :

$$e_g = 100 \times \frac{\sqrt{\sum_{i=1}^n (m_{exp}(i) - m_{th}(i))^2}}{\sqrt{\sum_{i=1}^n m_{exp}^2(i)}} \tag{6}$$

This allows us to determine the accuracy of the identified mass diffusivity.

### Results and Discussion

Experimental data were used to perform the inverse method. An excellent agreement found between the measured and the simulated curves of mass values on the optimal identified parameters is shown in Fig. 6. Table 1 shows the results obtained for each matched sample per species in radial and tangential direction at the minimum of objective function and the global relative error on each test. For the matched samples, the values of the diffusion coefficient are virtually similar. The little difference observed on certain sample is certainly due to the variability of wood. This shows that with this inverse method, the mass diffusivity value is accurately determined.



**Figure 6:** Measured and simulated mass at the optimum value of the diffusion coefficient identified for the sample 1 of European beech in radial direction

**Table 1:** Values of the estimated mass diffusivity

Wood species	Sample		D×10 <sup>10</sup> (m <sup>2</sup> .s <sup>-1</sup> )	Global error×10 <sup>3</sup> (%)
Violet wood	radial	1	1.90	8.89
		2	2.00	8.56
	Tange-ntial	1	1.00	6.30
		2	0.82	7.81
Ipe	radial	1	0.58	7.11
		2	0.56	8.91
	Tange-ntial	1	0.47	3.52
		2	0.41	3.49
European beech	radial	1	1.33	4.52
		2	1.30	14.94
	Tange-ntial	1	0.57	7.68
		2	0.48	9.65

Moreover, among the species studied, the mass diffusivity value of beech is most found in the literature. The comparison of our results (approximately 1.3×10<sup>-10</sup>m<sup>2</sup>/s in radial direction and 0.5×10<sup>-10</sup>m<sup>2</sup>/s in tangential direction) with the previous studies conducted with the same experimental device on beech shows that, those of [14] (1.5 ×10<sup>-10</sup> m<sup>2</sup>/s value of mass diffusivity in radial direction and 0.38 ×10<sup>-10</sup>m<sup>2</sup>/s in tangential direction) are little different while those of [15] are different (between 1.33×10<sup>-10</sup> and 0.99×10<sup>-10</sup> m<sup>2</sup>/s in tangential direction and a value about 2×10<sup>-10</sup> m<sup>2</sup>/s in radial direction). This is certainly due to the neglected of the coupled between heat and mass transfer in the analysis of experimental data of these studies.

Other studies such as [23] have given interesting results on effect of density and bound water moisture on wood mass diffusivity. This study has used a computational heterogeneous drying model to predict the mass diffusion coefficient in the wood. Indeed, for a density of 600 Kg/m<sup>3</sup> (approximately, that of beech) and bound water moisture between 10 and 15 %, their mass diffusivity value is between 0.7 and 0.9×10<sup>-10</sup>m<sup>2</sup>/s in radial direction and between 0.4 and 0.8×10<sup>-10</sup>m<sup>2</sup>/s in tangential direction. Our results on beech are not so far from these intervals.

A moment ago, [24] have determined beech mass diffusivity in unsteady-state by using a magnetic suspension balance. The values of 0.88×10<sup>-10</sup>m<sup>2</sup>/s and 1.02×10<sup>-10</sup>m<sup>2</sup>/s were found in absorption and in tangential direction respectively at equilibrium moisture content of 9.1 and 13.4% which approximates our measured interval. The high value of their results is certainly due to the measured temperature which is fixed on 50°C.

To ensure that the duration of 24 hours set by test is sufficient for reliable mass diffusivity identification, we realized a test of 36 hours on European beech in radial direction. The diffusion coefficients identified for different experimental durations remain almost constant between 10 and 25 hours (Fig. 7). This result shows that a minimum duration of 10 hours may even be sufficient to validate a test. That constitutes an additional gain in duration of experience. Such a progress could not be achieved without the use of numerical tools. Note that the similar experiment can take 10 days for the previous methods [15].

Before 10 hours, mass-diffusivity value increases quickly with the experimental duration. The gap between mass-diffusivity identified for duration of 1 hour and 10 hours is about 21%.

This proves that the transient mass-diffusivity of wood couldn't be determined at short time. In other hand, after

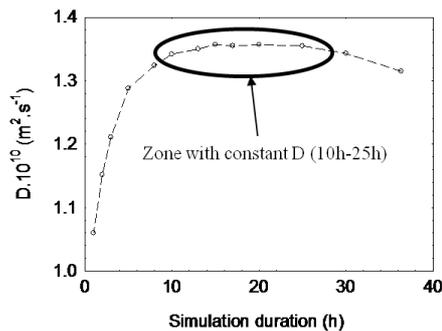


Figure 7: Effect of experimental duration on identified mass-diffusivity

25 hours, mass-diffusivity value decreases slowly with the experimental duration. The gap between mass-diffusivity identified for duration of 15 hours and 36 hours is about 3%. This was very little for a parameter of that kind.

## Conclusions

This study has shown that, besides the simulations of coupled heat and mass transfer in porous media, the code *TransPore* help estimate the bound moisture diffusion in the wood. This was possible due to not only the performances of the inverse method but also to the originality of experimentation. The calculation method, based on the code *TransPore* and a minimization of the deviation between the experience and simulation by simplex algorithm, has allowed to have a good accuracy on the diffusion coefficient and to reduce the duration of the simulation and the experiment. The excellent agreement between the calculated and the measured weight may estimate the effectiveness of this method.

The main advantage of this method was in the rigorous analysis of experimental data. Indeed, this rigour is characterized by the taking into account of the resistance of mass and heat transfer on the exchange sides of sample, the coupled between heat and mass transfer and especially real climatic conditions were undergone by the samples.

We can therefore conclude that the method developed in this study is distinguished from previous methods (analytical or numerical) at several points:

- The simulation is done with the help of the code *TransPore* which takes into account the coupled of heat and mass transfer as well as the actual climatic conditions of the experiment;
- A minimum time of 15 hours is enough to test a sample while it takes at least 10 days for a single test with the old methods (but the initial time of samples stabilization can be relatively long);
- Besides the moving of the sample from one climatic chamber to another, no further action of the operator is required throughout the identification process.

These qualities confer to this method, major strengths: reliability, rapidity and routine measurement.

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