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Experimental and ANN Estimation of the Mechanical Behavior for Cork under the Influence of Heat Treatment in Isothermal Conditions

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Abstract

The evaluation of the durability of the materials of thermal or acoustic isolation in the building walls in wet environment requires the study of the mass diffusivity in these walls. The primary objective of this work is to study and modelise the effect of high temperature treatment on the isothermal mass diffusion coefficient in cork. Using the indirect method of vaporimetric measurement yielded a radial diffusion coefficient D_R which increases with the temperature (35, 40 and 45°C), decreasing nine times after treatment (230°C), and causing a decrease in density. The experimental data base is used for an Artificial Neural Network (ANN) to estimate the diffusion coefficient where the mathematical model correlates the two input variables (state of treatment temperature and time) with D_R. The optimal ANN '*MLP*' whose architecture is (3-10-12-1) gave *AARE* = 0,098 and a correlation coefficient close to 1.

Keywords: Diffusion coefficient, Modeling, Cork, High Temperature Treatment

1. Introduction

For effective prevention of the condition of cork and the evaluation of its lifespan with good features in buildings and even in the process of storage, it is important to characterize the morphology in order to understand the flow of water steam in its pores. For the cork industry, it has been frequently noted that the measurements of these coefficients are of paramount importance for both energy consumption and drying cycle for the high temperature treatment [6], for modeling the hygroscopic behavior of cork, because the heat treatment of cork by mild pyrolysis is used to improve some of the characteristics of the final cork product, such as, its durability and dimensional stability [9]. It is therefore very important to know the influence of heat treatment at high temperature material in the mass transfer coefficient, as well as changes in physical and chemical properties over time, to allow on one hand, if biodegradation likely to occur or not and to allow the optimization of the treatment cycle on the other hand. Several studies have been performed on mass transfer in various materials such as wood [3]. They are sparsely presented in the literature [5; 7].

In this study, experiments are conducted in this direction to determine the coefficient of external mass transfer vaporimeter method, where the treatment effect is quantified by monitoring the desorption kinetics in a transient through a porous anisotropic medium under isothermal conditions in a tropical essence of cork from Algeria, in the radial direction before and after heat treatment. The experimental database is used to develop a methodology that will be used to determine the diffusion coefficient by a statistical approach based on artificial neural networks (ANN).

2. Materials and methods

The experimental protocol consists of a preparation of cork chips according to the geometrical aspect that fits the size of the vaporimeter vase with a radial direction (Figure. 1).

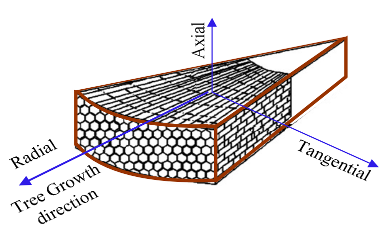

Figure 1: Illustration of the three main directions

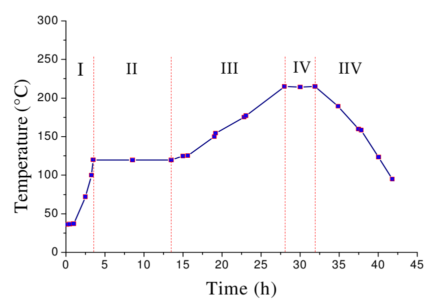

Figure 2: Typical heat treatment schedule

The three lots are heat-treated according to the cycle shown in figure.2 [2]. The other three lots are dried in an oven at 105°C. This process causes a decrease in the density ρ ($kg.m^{-3}$).

Dissemination in the cork is the process by which water migrates in two different shapes: (a) bound adsorbed water to the cell walls by intermolecular forces, namely H-bonding, (b) free water contained in the structural voids it is more difficulty to remove the bound water because the cell wall more affinity with water. The hygroscopicity of the different cell wall components is different taking into account the chemical characteristics of their molecular structures. During the process of diffusion of water, a difference in concentration between different cell layers is established. The water then migrates from a concentration gradient. The pressure gradient of water vapor [3] and the concentration gradient of water are expected to play an important role in the forces of water transport through the pores of cork. This distribution is dominated by the concentration gradient in water. This distribution is governed by Fick's first law. The flow rate is proportional to the concentration gradient.

$$J = -D\frac{\partial c}{\partial z} \quad (1)$$

On the other hand the second law of Fick takes into account the temporal dependence.

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial z}\left(D\frac{\partial c}{\partial z}\right) \quad or \quad \frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial z^2} \quad (2)$$

Where J is the flow of the considered parameter through cork, $\partial c/\partial z$ is the gradient of water concentration; C is the concentration and D the diffusion coefficient.

The diffusion depends on operating conditions such as the direction of diffusion and temperature and condition of the material to which the study sample is subjected [3]. These parameters must be considered in the measurement of diffusion coefficients of cork. Indeed, the variation of moisture content changes the conductivity of cork. From the measurements of the conductance of cork that allow the water content, we can deduce the diffusion coefficient.

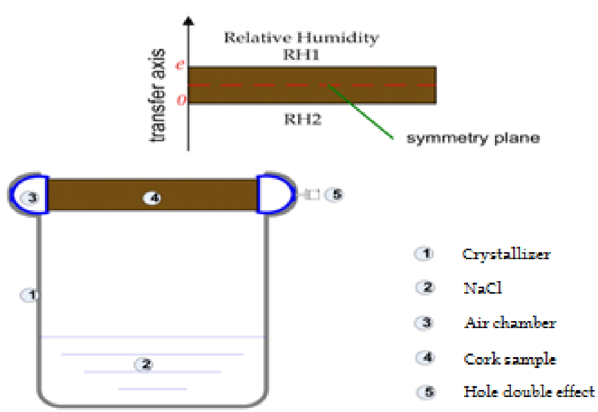

Figure 3: vaporimeter schematic

The experimental protocol employs the indirect method of vaporimeter (Figure.3), whose principle of measurement is based on steady-state technique vaporimeter, placed on a balance [8]. This type of experiment allows to calculate the diffusion coefficient of water in a given direction and temperature. We used a tracer *NaCl* (*0.2M*) to maintain constant relative humidity in an oven at temperatures of 35, 40, 45°C.From the mass change with time, we can quantify the the flow of moisture from the water through cork, that is:

$$\emptyset = \frac{dm}{dt} \tag{3}$$

According to Fick's first law, we deduce the diffusion coefficient.

$$D = j\frac{dx}{\Delta C} = \frac{\Delta x.\Delta m}{S.\Delta C.\Delta t} \tag{4}$$

ΔC is the difference in water concentration between the solution and the wood sample. Δx is the distance the specimen the solution *NaCl*.

In this permanent regime, the sample is weighed and dried in the oven at 105°C, it is again more weighed. The water concentration is given by the following equation:

$$C_e = \frac{\Delta m}{V} \tag{5}$$

Where: Volume sample is $V = e.S$ with *e* the thickness.

3. Implementation of ANN

We develop a methodology to estimate the D_R in cork, depending on the operating conditions mentioned in the experimental section using a statistical approach based on ANN, predictive technique used to benefit its parsimony and simplicity [1]. With this in mind, we set up an experimental database, of combining the morphological characteristics of cork (direction of diffusion), The State of treatment and time.

The main objective is to design an optimal network that must relate to the most appropriate number of layers and the number of hidden neurons adapted to our case.

4. Results and Discussion

The degradation of cork is highly dependent on temperature and mass losses become significant at 115°C (19% of initial dry weight) and increase rapidly for higher temperatures (36.4% at 230°C) the initial weight. The polysaccharides are the most heat sensitive components: at 200°C, hemicelluloses disappear and cellulose is degraded to a considerable extent.

Figures 4.(a, b and c), show the evolution of the mass of vaporimeter with time for both radial samples before and after treatment at temperatures of 35, 40 and 45°C. Based on experimental data collected and the surface of the sample that is the size of the vaporimeter cover, it is easy to compute D_R using equation 4.

The diffusion coefficient at baseline D_{RW} is 9 times larger than the diffusion coefficient of D_{RA} after treatment, due to the narrowing of the pores and the destruction of some chemical chains that increase the tortuosity.

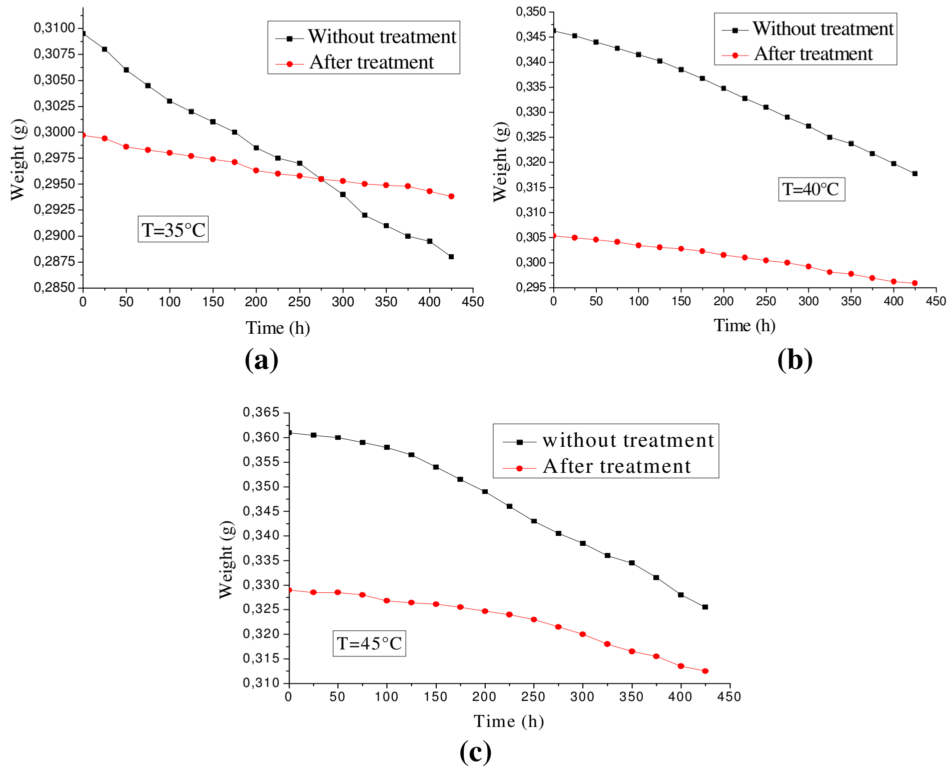

Figure 4: Evolution of the vaporimeter weight with and without treatment

We note that the coefficients respectively D_{RW} and D_{RA} are in the range of 10^{-11} and10^{-12} as they increase with temperature (Table.1), these results are consistent with theoretical predictions. In general, the diffusion coefficient increases with temperature according to a type Arrhenius equation.6, this is in agreement with the predictions of Magalhăesa (2008) for cork and Kermezli (2008) for wood.

$$D = D_0 exp\left(\frac{E}{RT}\right) \quad (6)$$

Where E is the activation energy (kJ mol^{-1}), R the gas constant (8.81 J mol^{-1}) and D_0 a constant that was estimed experimentally for cork as 4.0 m^{2}s^{-1}.The activation energy for diffusion of water was estimated as E=64kJ mol^{-1}[6].

Table 1: Diffusion coefficients of cork in isothermal conditions

Temperature	35°C	40°C	45°C
D_{RW} (m^2s^{-1})	4.67x10^{-11}	6.44x10^{-11}	8.19x10^{-11}
D_{RA} (m^2s^{-1})	5.12x10^{-12}	7.06x10^{-12}	9.21x10^{-12}

The model, ANN (*MLP*) optimized illustrated, is given by an architecture (3-10-12-1).

For all phases of test and generalization studied, the correlation coefficient is R = 1.0000. This result confirms the robustness of the neural model established and the possibility of predicting the various parameters that characterize the mass diffusion in anisotropic porous media. To make the comparison between experimental results and those predicted by ANN, wettest the *MLP* with another data base, not used in the learning chain-validation. The *MLP* was able to predict our settings with great performance (Table 2).

Tableau 2: Statistical performance of ANN

ANN	AARE (%) Test cases	AARE (%) generalization	MAE (%) Test cases
Diffusivity	0.090	0.089	0.041

5. Conclusion

We were able to measure and estimate the radial diffusion coefficient of water vapor in cork under isothermal conditions as a result of treatment condition. In the field hygroscopic cork, the diffusion coefficient increases with temperature and at the same temperature coefficient decreases for the treated material to 9 times the D_R untreated cork.

These results may be useful for modeling the industrial drying of cork. The neural model developed whose structure (3-10-12-1), is able to predict with great accuracy the diffusion coefficient of mass before and after treatment (*MAE* does not exceed 0.041%). The mass diffusion coefficient of the cork will be included in the calculation code governing the mass transfer in cork.

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