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Mass Transfer in an Anisotropic Porous Medium-Experimental Analysis and Modelling of Temperature and Desorption Direction Effect

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Abstract

In order to follow the kinetics of desorption of the aqueous solution (KCl “0.2M”) which occur in three orthotropic directions, this work uses the indirect method of conductimetric measurement. An anisotropic porous medium which consists of beechwood in form of plate is examined at various temperatures, ranging from 20°C to 40°C.

Including simplifying assumptions, the equation of mass is solved using Laplace transforms, in the first step. Starting from the law of Nernst – Einstein, the resulting system of equations enables us to determine Dapp (apparent coefficient of diffusion of the aqueous solution) and tortuosity. Based on Arrhenius relationship, the analysis of the temperature effect on the kinetics of desorption makes it possible to propose empirical correlations between temperature and the aforementioned parameters.

In the second step, the total coefficient of the external mass transfer in transient state is estimated by adopting two approaches: One using a total assessment of static transfer mass and the other, using total assessment of surface mass transfer.

Keywords: Kinetics of desorption; Anisotropic medium; Porosity; Modelling; Tortuosity; Total coefficient of transfer of matter

1. Introduction

As it is, non-homogeneous and it is characterized by an important anisotropy, wood is a very complex material. It is also a hygroscopic material: its water content varies with time according to humidity conditions, temperature, environment and the nature of soil [3]. it is thus very important to know the concentration of the chemical species diffusing in the material as a whole and locally, as well as its variations with time, in order to predict whether biodegradation occurs on one hand, and on the other hand, to allow the consumption of reagent during dry-up to be optimized. Several studies were carried out on the mass transfer in various wood types [5,2]. They are presented in the literature in a scattered way. They differ in the approach targeted by each study. Carried out studies, taking account of low temperature, have not been found in literature.

In this study, experiments are carried out in order to determine the tortuosity and the global coefficient of external matter transfer.

Unlike conventional studies undertaken with pure water [1], the nature of aqueous solution will be varied with respect to the dissolved chemical species. This work is based on the indirect method of conductimetric measurement for following the kinetics of desorption of the aqueous solution (KCl “0.2M”). This method has been revealed very simple in its material conception, highly accurate and the results thereof immediately obtainable. The aqueous solution diffuses radially, tangentially and longitudinally within an anisotropic porous medium (beechwood in form of plate) towards an external environment at various temperatures ranging from 20°C to 40°C.

The kinetics of desorption of the aqueous solution in the porous medium is modelled and the deduced equation of mass is solved by using Laplace transforms and by adopting some simplifying assumptions as well as appropriate boundary and initial conditions. Then, a simplified solution will be obtained using the method of separation of variables.

2. Experimental set-up

Experimental set-up is illustrated in Figure 1. It consists, firstly, of preparation of shavings according to the geometrical, direction of cutting, drying aspects and according to their masses. Secondly, the impregnation of beechwood in an aqueous solution (KCl or NaCl) and finally, the shavings are introduced into initially distilled and ionized water (Figure 2). As the measurement of the evolution of the concentration represents the image of electric conductivity (eq. 4), the experiment is repeated at a number of different temperatures in the radial, longitudinal and tangential directions.

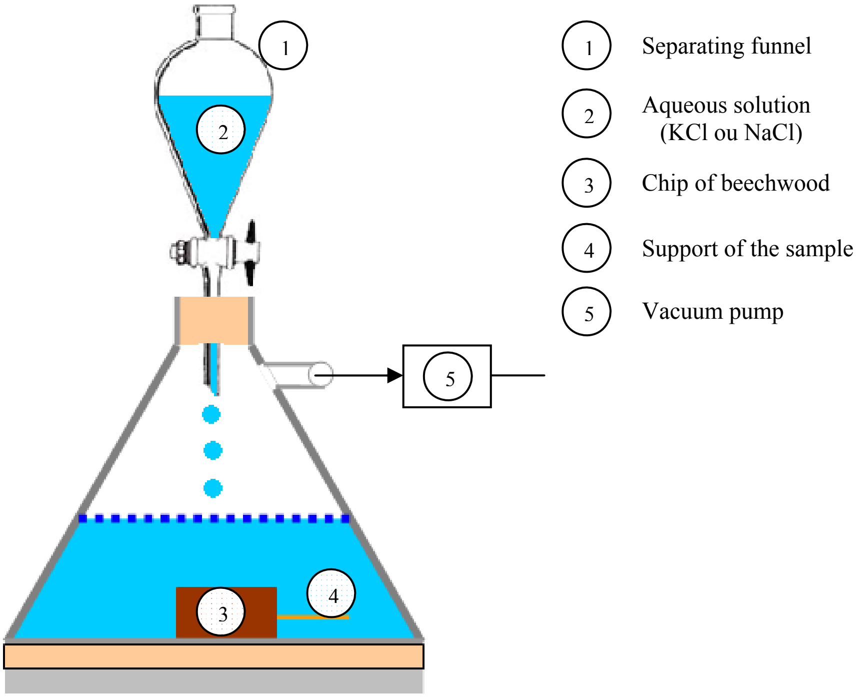

Figure 1: Illustration of the vacuum impregnation of the sample

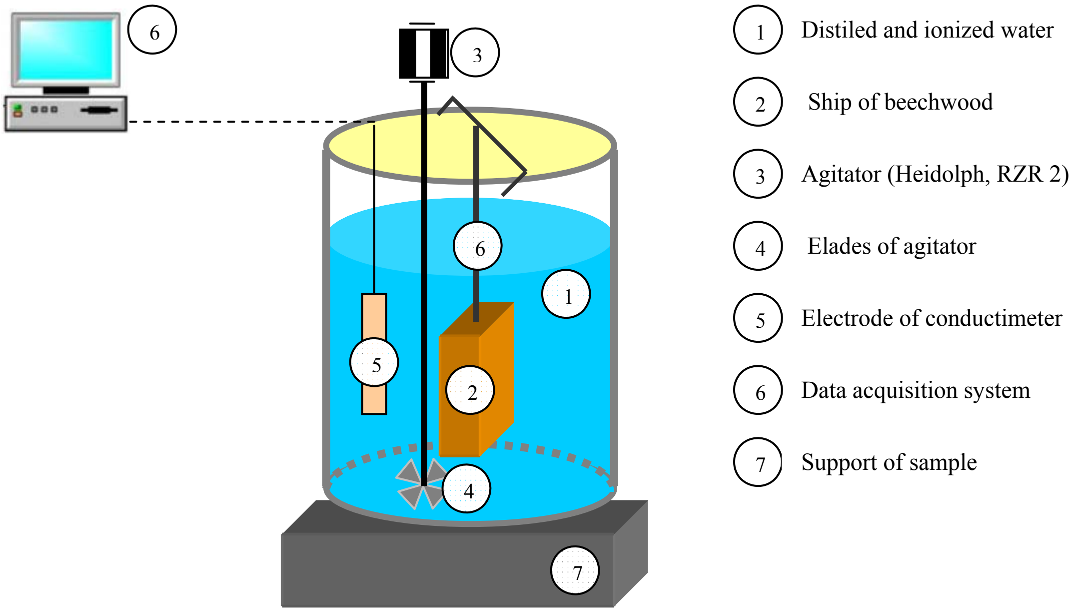

Figure 2: Illustration of the measurement of concentration of desorption.

In order to evaluate the mass diffusivity (D_X (cm^2/s)) as well as the concentration of the aqueous solutions towards the external medium, computations based on these experiments using the following expressions from Nernst – Einstein [4], are given:

$$D_{K^+Cl^-/H_2O}=\frac{RT}{F^2}\cdot\frac{\frac{1}{Z_{Cl^-}}+\frac{1}{Z_{K^+}}}{\frac{1}{\lambda^0_{Cl^-}}+\frac{1}{\lambda^0_{K^+}}}=\frac{8.3143\cdot T}{96488^2}\cdot\frac{\frac{1}{1}+\frac{1}{1}}{\frac{1}{76.35}+\frac{1}{73.5}}=6.6891.10^{-8}\,T \qquad \textbf{(1)}$$

The conductivity of the fluid indicated by the conductimeter is given by the following :

$$\Lambda_{KCl}=\sum_i\left(\lambda_i\cdot z_i\cdot c_i\right)=\lambda_{K^+}\cdot c_{KCl}+\lambda_{Cl^-}\cdot c_{KCl}=c_{KCl}\left(\lambda_{K^+}+\lambda_{Cl^-}\right) \qquad \textbf{(2)}$$

Where: *R=8.3143 J/(mole.K)* the ideal gas constant , *F = 96488 (C)* the Faraday number, *T* the temperature of water *(K)*, λ_i equivalent conductivity of the ion "*i*" given by the extrapolated value for an infinite dilution, Z_i charge of the ion "*i*" in absolute value, Z_X the algebraic load (in absolute value) of the anion and/or the cation. c_i the concentration of ions (gr/l) and Λ_{KCl} the conductivity of the fluid measured by the conductimeter, Thus:

$$\begin{aligned}c_{KCl}(mM)&=\frac{\Lambda_{KCl}}{\left[\lambda_{K^+}(T)+\lambda_{Cl^-}(T)\right]}\\&=\frac{\left(\Lambda_{KCl}\right)_t-\left(\Lambda_{KCl}\right)_{t=0}}{\left[\lambda_+^\infty+a_+(T-25)+b_+(T-25)^2+c_+(T-25)^3\right]+\left[\lambda_-^\infty+a_-(T-25)+b_-(T-25)^2+c_-(T-25)^3\right]}\end{aligned} \qquad \textbf{(3)}$$

The fluid concentration in function of time, is attained at through electric conductivity, thus:

$$\begin{pmatrix}\text{Concentration of desorption}\\ \text{of the(i) to time(t)}\end{pmatrix}=\frac{\begin{pmatrix}\text{Conductivity of the (i) measured}\\ \text{by the conductimeter to time(t)}\end{pmatrix}-\begin{pmatrix}\text{Initial conductivity of the (i) } \textit{measured}\\ \text{by the conductimeter to temps(t = 0)}\end{pmatrix}}{\begin{pmatrix}\text{Cationic equivalent conductivity}\\ \text{to the température (T)}\end{pmatrix}+\begin{pmatrix}\text{Anionic equivalent conductivity}\\ \text{to the température (T)}\end{pmatrix}} \qquad \textbf{(4)}$$

Where: λ^0_X equivalent conductivity limits diffusion of the anion and/or cation in water at *25°C.*

3. Modelling

3.1. Physical model

The composite material has an initial concentration (c_0), it is located in a well-mixed solution of concentration (c_∞). The coefficient of surface mass transfer (k) is very significant so that the surface concentration (Cs) remains constant. The latter is equal to (C^*) as soon as the process begins $(C^* = k_p.\ c_\infty)$.

3.2. Simplifying assumptions

To reduce and to simplify the mathematical analysis, the following simplifying assumptions are necessary:

- Absence of chemical reaction and adsorption of the aqueous solution.
- The porous medium (the wood shavings) is homogeneous.
- The distribution of the initial concentration is uniform within the composite.
- The convection is disregarded (perfectly mixed medium).
- The transfer is one-dimensional (isolated faces).
- The physicochemical properties of the composite (diffusivity) and/or the fluid are independent of the concentration, space, moisture and time [6].
- The surrounding medium is assumed to have finite volume. The solution concentration is negligible in comparison with the concentration in the internal medium.

3.3. Mathematical model

Here, we develop equations for determining the concentrations inside the composite. They rely on the mass balance of the diffusing chemical species *(i)* which diffuses through a differential volume element *(dv)* of the composite, according to the mass transfer equation for various geometries of composite. The dimensionless problem has been considered, using the appropriate simplifying assumptions.

4. Objects in the form of plates

The considered shaving has three orthotropic directions shape (cut longitudinally, radially and tangentially) of a plate (Figure 3).

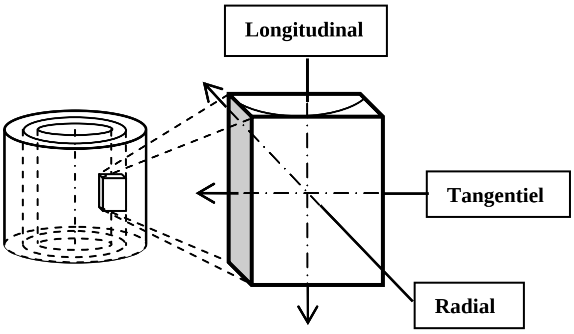

Figure 3: Various directions of flow

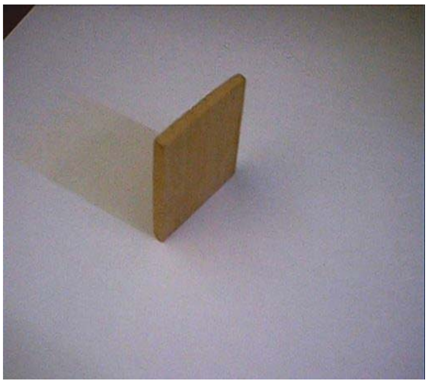

Figure 4: Photograph of the plate of beechwood used

Table 1: Experimental data of the beechwood shavings in the form of plates directed in 90 °

	Siccity S (%)	*Side* *(m)*	*Thickness* e_H*=2l (m)*	*Porosity* *ε*	*Soluty* *KCl (M)*
Plate n°1 Longitudinally	91	$34.5\ 10^{-3}$	$6.00\ 10^{-3}$	0.674	0,5
Plate n°2 Radially	90	$34.5\ 10^{-3}$	$6.00\ 10^{-3}$	0.671	0,5
Plate n°3 transversally	89.5	$34.5\ 10^{-3}$	$6.05\ 10^{-3}$	0.675	0,5

The system to be solved according to the simplifying assumptions, to the boundary conditions and to the initial condition takes the following form:

$$\left.\begin{aligned} & D_{i\,app}\frac{\partial^2 c_i(x,t)}{\partial x^2}-\frac{\partial c_i(x,t)}{\partial t}=0 \\ & c_i(x,t)\Big|_{t=0}^{x>0} = c_{i0} \\ & c_i(x,t)\Big|_{t>0}^{x=l} = c_{ip} \\ & \frac{\partial c_i(x,t)}{\partial x}\bigg|_{t>0}^{x=0} = 0 \end{aligned}\right\} \qquad (5)$$

The solution of the preceding system is:

$$\frac{c_i(x,t)-c_{i0}}{c_{ip}-c_{i0}}=1-\frac{4}{\pi}\sum_{n=0}^{\infty}\left\{\frac{(-1)^n}{(2n+1)}\cos\left(\frac{(2n+1)\cdot\pi}{2l}\cdot x\right)\cdot\exp\left(-\frac{(2n+1)^2\cdot\pi^2\cdot D_{i\,app}}{4l^2}\cdot t\right)\right\} \quad \textbf{(6)}$$

Or:

$$\frac{m_t}{m_\infty}=1-\frac{8}{\pi^2}\sum_{n=0}^{\infty}\left\{\frac{1}{(2n+1)^2}\cdot\exp\left(-\frac{(2n+1)^2\cdot\pi^2\cdot D_{i\,app}}{4l^2}\cdot t\right)\right\} \quad \textbf{(7)}$$

Where: c_i concentration of the chemical species *(i)* diffusing *(mol/m^3)* and *Diapp the* diffusivity of *(i)* apparent. m_t mass of the substance released at time *t*, m_∞ mass substance transferred after total desorption from the shaving after an infinite time; *Ci* reduced concentration $\{C_i = (c_i - c_{i0}) / (c_{ip} - c_{i0})\}$

5. Results and discussions

The previously established expressions enable us to determine, the Dapp along with the tortuosity after the computation of D_A [7] (effective diffusivity for KCl) starting from Nernst-Einstein's law [4].

$$D_A = 6.6891.10^{-8}\,T \quad \textbf{(8)}$$

$$D_{app} = D_A \cdot \frac{\varepsilon}{\tau^2} \quad \textbf{(9)}$$

We focus here on the effect of temperature and direction of the desorption of aqueous solution in the shavings of beechwood. Figure 5 shows the evolution of the concentration against time for various temperatures. Furthermore the experimental data are reported in Table 2.

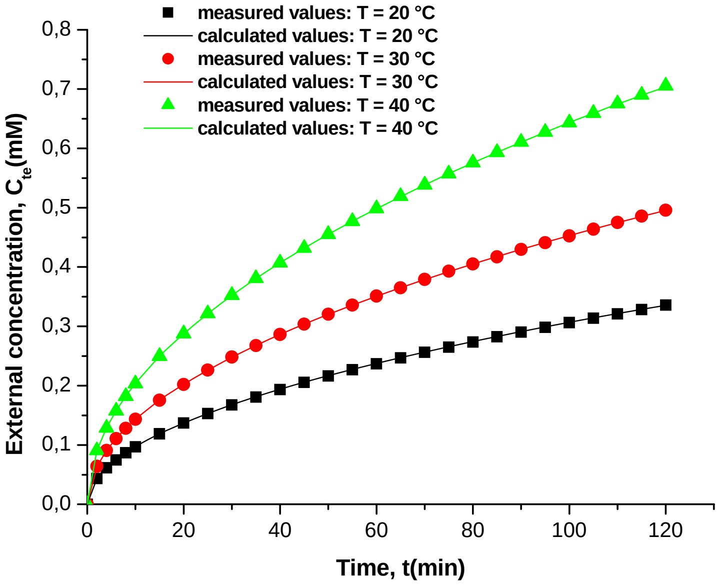

Figure 5: Effect of temperature on the evolution with time of external concentration.

We note that the higher the temperature is, the higher the desorption is of a favorable effect. It is also seen that the experimental results and those of numerical modelling are in perfect agreement.

Based on Arrhenius relationship [6] and according to this validation it is possible to control D_{app} as well as the tortuosity τ in function of porosity ε.

The post-processing made it possible to propose two empirical correlations, the first, is a relationship between D_{app} and the temperature, whereas the second is an expression between tortuosity and temperature.

$$D_{app} = 0,99 \exp\left(\frac{-3153,63}{R\,T}\right) \tag{10}$$

$$\tau = 3,603.10^{-5} \exp\left(\frac{3434,19}{T}\right) \tag{11}$$

Table 2: Values of effective, apparent diffusivity and of tortuosity according to the temperature

	Interval of ***t (min)***	***Dapp*** ***(m^2/S)***	***D_A*** ***(m^2/S)***	**Tortuosity**	**Temperature** ***(°C)***
Radial plate Beechwood *KCl (0.2M)*	[0 – 120]	$0.70.10^{-10}$	$1,961.10^{-9}$	4,393	20
	[0 – 154]	$1,03.10^{-10}$	$1,994.10^{-9}$	3.619	25
	[0 – 120]	$1,50.10^{-10}$	2,028.10-9	2.996	30
	[0 – 120]	$2,18.10^{-10}$	$2,061.10^{-9}$	2,491	35
	[0 – 120]	$3,11.10^{-10}$	$2,095.10^{-9}$	2,079	40

In the second step the total coefficient of the external mass transfer in transient state is considered by adopting two approaches:

- Using the global balance of static mass transfer:

$$k = -\frac{v_l\, v_v}{(v_v + v_l)\, S\, t}\, ln\left(1 - \frac{(v_v + v_l)\, c_i}{v_v\, c_{i0}}\right) \qquad \textbf{(12)}$$

- Using the global balance of surface mass transfer:

$$k = \frac{4\, D_{i,app} \cdot (c_{i,0} - c_{i,p})}{(c_{i,p} - c_{i,t}) \cdot e_H} \sum_{n=0}^{\infty} \left\{ \exp\left(-\frac{(2n+1)^2 \cdot \pi^2 \cdot D_{i\,app}}{4\, l^2} \cdot t \right) \right\} \qquad \textbf{(13)}$$

Where: v_v *the* volume of the vacuum, c_{i0} initial concentration of *i*, v_l *the* volume of the aqueous solution, $c_i(t)$ of the concentration instantaneous of *i* external, *(e_H) the* thickness of the shaving.

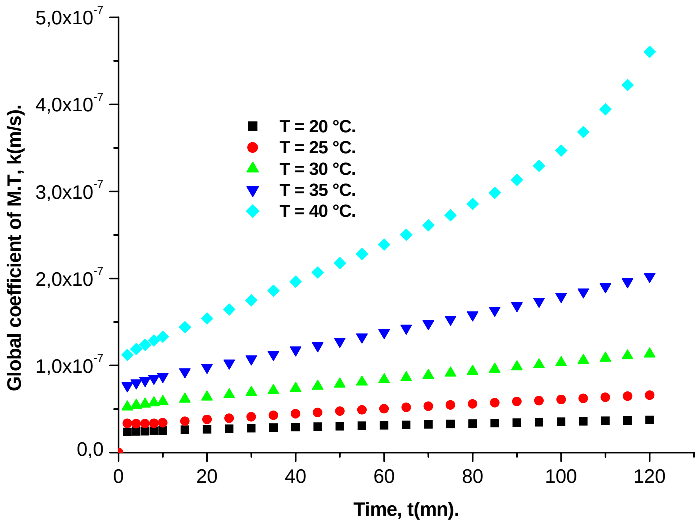

Figure.6: Variation of mass transfer (MT) global coefficient with time Temperature effect

To substantiate the verification, Figure 6 shows the temperature effect on the variation of mass transfer (MT) global coefficient with time. It is clearly seen that time has a little influence on the D_{aap} for temperatures below 35°C. However, for T=40°C, this coefficient increases in parabolic way.

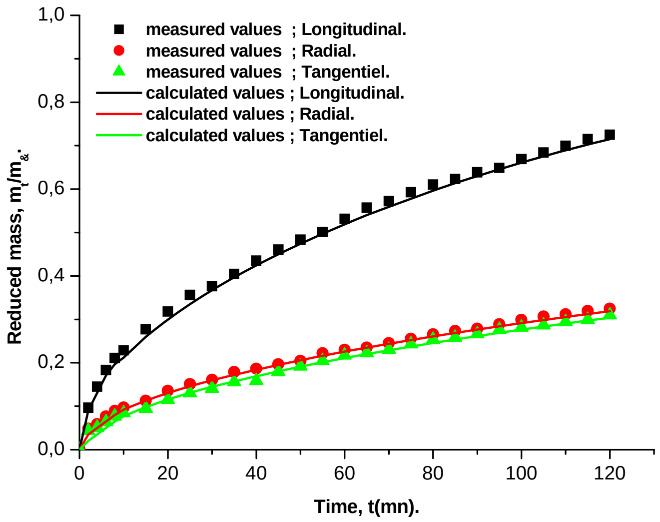

Figure 7: Variation of reduced mass against time effect of diffusion direction

We can therefore conclude that the model we have presented is able to simulate desorption kinetics very satisfactorily. Desorption of the solute has been found favorable in the longitudinal direction than in the radial and tangential directions. This, because the longitudinal path followed by ions is less tortuous than those of radial and tangential directions. However, the high value of diffusion coefficient in the radial direction with respect to tangential direction can be attributed to wood shelves that do not exist in the tangential direction.

This demonstrates once again the importance of anisotropy of wood and its impact on the local and global characteristics.

6. Conclusion

The objective of this work is the study of the influence of solutions temperature and the material anisotropy on desorption of an aqueous solution, impregnating a porous medium.

The results that we have obtained, although enjoying many similarities with those attained at by many other authors, do have a large array of possibilities to cover many parameters, such as low temperature which has not been considered in the literature. In a more accurate and clearer scope, our results could be thus summed up.

1- Two empirical correlations were proposed, one connecting the apparent coefficient of diffusion to the temperature and the other the tortuosity to temperature.

2- Furthermore, our study showed the important effect of temperature below 40°C on the total diffusion coefficient.

3- Experiments and modelling have been carried out on a beechwood plate and allowed to determine the major parameters such as total coefficient of transfer of matter and the tortuosity of the medium.

Application of the obtained results with ANN method is being considered, and will be the subject of future paper.

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