

# A novel methodology for the rapid identification of the water diffusion coefficients of composite materials



M. Beringhier\*, M. Gigliotti

Institut P', CNRS – ISAE ENSMA – Université de Poitiers, Département Physique et Mécanique des Matériaux, ENSMA, Téléport 2, 1 avenue Clément Ader, BP 40109, 86961 Futuroscope Chasseneuil Cedex, France

## ARTICLE INFO

### Article history:

Received 3 July 2014  
Received in revised form 19 September 2014  
Accepted 30 September 2014  
Available online 13 October 2014

### Keywords:

A. Polymer–matrix composites (PMCs)  
B. Environmental degradation  
C. Numerical analysis  
C. Computational modelling

## ABSTRACT

The paper presents a novel methodology for the rapid identification of the water diffusion coefficients of composite materials. The methodology consists in employing a numerical parametric Proper Generalized Decomposition (PGD) method allowing incorporating the diffusion coefficients among the number of degrees of freedom. Compared to classical identification schemes, often based on Finite Element Method (FEM) iterations, the proposed method allows achieving consistent CPU time gain. The method is general and can be applied when diffusion anomalies take place or when diffusion–reaction coupling must be taken into account, moreover can deal with anisotropic materials. However, for the scope of illustration, in the present case, it is applied to the simple case of “classical diffusion” (Fick’s model with constant boundary conditions) and concerns isotropic materials.

© 2014 Elsevier Ltd. All rights reserved.

## 1. Introduction

Composite materials are more and more employed in the aeronautic and automotive industry for the realization of structural parts. These structures may be exposed to the environment over long times, leading to durability and ageing issues. In particular water diffusion in polymer matrix composite materials may promote material degradation, residual strength reduction, lowering of the glass transition temperature of polymer matrices, global decrease of the material performance [1]. A vast literature exists on the subject, concerning the study of water diffusion mechanisms within the macromolecular polymer network [2–4,1], the effect of water on the mechanical properties of matrices [2,1] and composites [5,1], modelling water transport within the material according to thermodynamics [6,7] or theory of mixtures [8] based models of diffusion. In many practical situations, it is very important to be able to predict with good accuracy not only the maximal amount of water which can ingress the composite material but also the speed at which water diffusion takes place with the aim of establishing the water diffusion kinetics within the material: in other words, one may be interested in characterizing the sorption capabilities and the diffusivity of the material. A good way to access this information is to perform a so called sorption test: during this test a material sample is exposed to a

humid environment (with fixed relative humidity, RH) at a given temperature and periodically weighted to get a gravimetric curve. A schematic shape of several different gravimetric curves is resumed in Fig. 1 (this scheme is taken from [1], in which the transient weight of absorbed water over the entire volume of the sample,  $m_w(t)$ , divided by the maximum weight of absorbed water,  $m_{w_\infty}$ , is plotted against the square root of time ( $\sqrt{t}$ )).

Curve LF in Fig. 1 represents Linear Fickian (LF) behaviour: in this case, the amount of water increases linearly with  $\sqrt{t}$  during the first phases of the sorption test, then the sample gets a stable saturated state (saturation plateau) in which  $m_w(t)$  equals  $m_{w_\infty}$ , that is, the ratio  $m_w(t)/m_{w_\infty}$  becomes equal to 1. For materials which behave according to the LF curve, there exists a maximum amount of absorbable water, moreover diffusion kinetics is linear (with respect to  $\sqrt{t}$ ) in the transient state. Gravimetric curves of type A, B, C and D are often referred as anomalous with respect to LF behaviour; diffusion anomalies may be related to diffusion–reaction phenomena (such as hydrolysis of the polymer network and chemical ageing [1], Langmuir or two-stage sorption behaviour [9,4], interaction between water and the viscoelastic polymer network (relaxation [6])). In several cases water diffusion follows the simple LF behaviour and the Fick’s law gives a good approximation of the diffusion kinetics. According to the Fick’s model the amount of water absorbed by an initially dry parallelepipedic sample (with length  $L_x$ , width  $L_y$  and thickness  $e$ ),  $m_w(t)/m_{w_\infty}$ , as a function of time is given by the following explicit expression [1]

\* Corresponding author.

E-mail address: [marianne.beringhier@ensma.fr](mailto:marianne.beringhier@ensma.fr) (M. Beringhier).

$$\frac{m_w(t)}{m_{w_\infty}} = 1 - \left(\frac{8}{\pi^2}\right) \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \sum_{p=1}^{\infty} \frac{1}{(2m+1)^2 (2n+1)^2 (2p+1)^2} \exp(Qt) \quad (1)$$

where  $Q$  writes

$$Q = \pi^2 \left( D_{xx} \left(\frac{2m+1}{L_x}\right)^2 + D_{yy} \left(\frac{2n+1}{L_y}\right)^2 + D_{zz} \left(\frac{2p+1}{e}\right)^2 \right) \quad (2)$$

in which  $D_{xx}$ ,  $D_{yy}$  and  $D_{zz}$  represent the diffusivity parameters of the material along directions  $x$ ,  $y$  and  $z$  respectively. These parameters may depend on temperature, since the diffusion mechanisms are likely to follow an Arrhenius-like behaviour. This dependency is however neglected in the present case. Eq. (1) is written under the hypothesis that the material is orthotropic (with respect to diffusion) and that  $x$ ,  $y$  and  $z$  are the principal directions of orthotropy. Moreover, the boundary conditions along the external surface of the sample are taken as uniform and constant and the initial condition is null. If  $D_{xx} = D_{yy} = D_{zz} = D$  (isotropic material), Eq. (1) takes a simpler form. Some further details about the derivation of Eq. (1) will be given in Section 2 and can be found in [1]. As far as the identification is concerned, besides the maximum amount of absorbable water ( $m_{w_\infty}$ ), one deals with three parameters ( $D_{xx} \neq D_{yy} \neq D_{zz}$ ) in the orthotropic case, while the number of diffusion parameters reduces to one ( $D$ ) in the isotropic case.  $m_{w_\infty}$  can be directly read (inferred) by the gravimetric curves (saturation plateau), the diffusion parameters must be inferred (identified) by comparing the experimental with simulated curves (Eq. (1)). It should be noted that, as a matter of fact, at least three gravimetric curves are needed to establish the diffusion parameters in the orthotropic case, while one curve suffices in the isotropic case. The diffusion parameters of the Fick's law have been identified by means of Eq. (1) in [10,11], for both isotropic and orthotropic materials, by minimizing the error between the simulated and the experimental gravimetric curve. LF behaviour can be also simulated by numerical methods, e.g. the Finite Element Method (FEM) [1]; in this case the diffusion parameters can be extracted by iterating the numerical solution up to convergence between experiments and simulation for different values of the diffusion parameters [10,11,1]. Re-update of FEM solution represents a classical identification procedure which must be employed when analytical explicit solutions are not available, that is, for instance, in the presence of LF behaviour for domains which are not parallelepipedic, cylindrical or spherical [1], or in the presence of anomalous behaviour (non-LF behaviour), when diffusion–reaction couplings take place or anomalous (non-uniform or non-constant) boundary conditions have to be employed. For a given value of the diffusivity parameter, the absorption curve is determined by extracting from the model the evolution of the total amount of absorbed water. The fitting error  $Res(t_i)$  at each time  $t_i$  is defined as follows:

$$Res(t_i) = \frac{M^{MODEL}(t_i) - M^{exp}(t_i)}{\langle M \rangle} \quad (3)$$

where  $M^{MODEL}(t_i)$  is the volume of water calculated by the model for a given value of the diffusion parameters,  $M^{exp}(t_i)$  is the experimental volume of water absorbed by the specimen, and  $\langle M \rangle$  is the average of the water volume content measurement. The residual which characterizes the errors due to the given value of the parameter at iteration  $j$  is defined by:

$$Res_j = \sum_i (Res(t_i))^2. \quad (4)$$

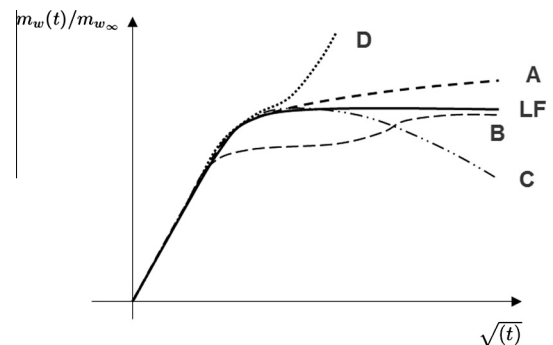
The successive diffusivity parameter at iteration  $j + 1$  is obtained by minimizing the residual with a non linear least squares solver, for instance. The optimal value of the parameter is obtained when

differences in two consecutive values of the parameters are less than a given threshold.

Classical techniques have major drawbacks: methods employing analytical solutions can be applied for samples with regular domains (parallelepiped, cylinder or sphere) and without diffusion anomalies (except in very specific cases [12]), methods employing FEM solution are often expensive from the computational point of view, since the cost of one FEM solution may be high, in particular in the presence of diffusion anomalies, diffusion–reaction coupling and generally nonlinear behaviour.

The paper presents a novel methodology for a rapid identification of the water diffusion coefficients of composite materials. The methodology consists employing a numerical parametric Proper Generalized Decomposition Method (PGD) [13] allowing incorporating the diffusion coefficients as extra-coordinates. This method is more efficient than classical identification schemes: it presents a higher degree of generality with respect to analytical formulas, since it can be applied when diffusion anomalies take place or when diffusion–reaction coupling must be taken into account; compared to FEM iterations, it allows achieving consistent CPU time gain. Moreover it can deal with anisotropic materials. This idea has been proposed by Chinesta et al. (see [14,13] and the references therein) and has been extended for other types of extra-coordinates as initial and boundary conditions [15,16], large number of process parameters [15] and more recently the length of the domain [17]. In [15], these authors have employed the parametric PGD solution for identifying and optimizing the thermal parameters involved in die thermal process: in this context, the computed temperature field can be directly compared to the measured temperature field which can be evaluated at several experimental points, allowing a robust identification.

As soon as moisture absorption is concerned, the identification of the diffusivity parameters is not so obvious. In fact, in this case, the calculated water concentration field cannot be directly compared with the measured one, since experimental techniques for measuring the full water concentration field are not currently available and one must rely solely on gravimetric curves. Therefore, the identification procedure must be performed by comparing the experimental sample mass with the computed one, which is obtained by integrating the parametric water concentration field over the spatial domain. We can notice that, for a given conditioning time, gravimetric curves represent a scarce number of experimental points, which constitutes an additional complexity for identification procedure. Consequently, the originality of the present contribution is not the implementation of the parametric PGD method but the evaluation of the efficiency of this method for this specific application having in mind that the identification is performed by employing an integrated field.



**Fig. 1.** Schematic illustration of a sorption test with several different gravimetric curves corresponding to different material responses to water absorption (the scheme is taken from [1]).

Download English Version:

<https://daneshyari.com/en/article/7892192>

Download Persian Version:

<https://daneshyari.com/article/7892192>

[Daneshyari.com](https://daneshyari.com)