Characterization of the diffusivity function through water-uptake tests

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Abstract. A method is proposed to determine the moisture diffusivity of capillary active materials by means of water-uptake tests performed with different initial water contents. The method is based on an analytical approach, in which the diffusivity is approximated as a multiple step function of the water content. Contrary to other well-established techniques, the method proposed here requires neither the knowledge of the water content distribution in the absorbing sample, nor the application of numerical simulations. Experiments are carried out on calcium silicate samples.

1 Introduction

The absorption of moisture in several capillary active materials obeys a diffusion law in which the transport potential is the water content and the material behaviour is described by the so-called diffusivity function, whose experimental characterization is generally complex and time consuming. In fact, the currently available experimental methods require an exact knowledge of the moisture profile in a sample subject to absorption or drying. Therefore, advanced measuring technologies such as nuclear magnetic resonance [1] or X-ray projection [2] are necessary. Alternatively, inverse procedures based on complex algorithms and numerical simulation, as the one reported in [3], can be used.

In this study, a different approach, which neither requires the knowledge of the water content distribution, nor the application of numerical simulation, is tested for the first time. The proposed method is based on the analytical model reported in Ref. [4] in which the diffusivity function is approximated as a multiple-step-function of the water content. This function is determined through a set of water uptake tests performed with different initial water contents. The procedure is carried out by starting from the highest water content level and decreasing step by step to the lowest one.

For this first test of the method, calcium silicate insulation samples are employed. This material, commonly used for internal insulation of buildings, is capillary active and highly homogeneous. It is therefore particularly suitable for these experiments.

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2 Description of the method

In this section, the mathematical model employed for inverse determination of the diffusivity function is described.

2.1 Mathematical model

We consider isothermal absorption in a porous material, homogeneous at the macroscopic scale, in which gravity is negligible when compared to the capillary forces. The three-phase system (solid matrix, humid air and liquid water) is assumed to be in local thermodynamic equilibrium at each instance of time. Hence, according to several authors ([1] and [2] among others), the one-dimensional moisture transfer in the material can be described by the following diffusion equation:

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x} \left(D(u) \frac{\partial u}{\partial x} \right) \quad (1)$$

Here, u denotes the local volumetric water content (-) and $D(u)$ the diffusivity function (m^2/s). The initial and boundary conditions are given by the following equations:

$$u(0, x) = u_0 < 1 \quad (2)$$

$$u(t, 0) = 1 \quad (3)$$

$$\lim_{x \rightarrow \infty} u(t, x) = u_0 \quad (4)$$

Note that, in general, the moisture diffusivity is steeply increasing with the water content, which is often approximated by an exponential function. Nevertheless, in this study we shall use a different approach by introducing the following multiple-step-function:

$$D(u) = \begin{cases} D_1: 0 < u < u_1^* \\ \vdots \\ D_i: u_{i-1}^* < u < u_i^* \\ \vdots \\ D_n: u_{n-1}^* < u < 1 \end{cases} \quad (5)$$

where the coefficients u_i^* denote the water contents at which the diffusivity changes. This approach is profitable since it allows to find analytical solutions of the above problem for arbitrary diffusivity functions. In particular, by applying the well-known Boltzmann transformation, it can be shown that the solution $u(t, x)$ is given by a set of n functions $u_i(\lambda)$, each one holding in a different water content region:

$$u(x, t) = u(\lambda) = \begin{cases} u_1(\lambda): 0 < u < u_1^* \\ \vdots \\ u_i(\lambda): u_{i-1}^* < u < u_i^* \\ \vdots \\ u_n(\lambda): u_{n-1}^* < u < 1 \end{cases} \quad (6)$$

with the variable λ defined as follows:

$$\lambda = \frac{x}{\sqrt{t}} \quad (7)$$

In **Fig. 1**, an exemplary curve $u(\lambda)$ and the corresponding water content profiles in an absorbing sample are represented. Here, the λ_i^* values denote the boundaries of the different water content regions in which the diffusivity is constant. At these boundaries, the continuity conditions

$$u_i(\lambda_i^*) = u_{i+1}(\lambda_i^*) = u_i^* \quad (8)$$

and

$$D_i \frac{du_i}{d\lambda}(\lambda_i^*) = D_{i+1} \frac{du_{i+1}}{d\lambda}(\lambda_i^*) \quad (9)$$

hold.

Fig. 1. Exemplary curve $u(\lambda)$, and water content profiles $u(x, t)$ in an absorbing sample.

2.2 Inverse determination of the diffusivity function

According to the model introduced above, the following equation holds for an arbitrary initial water content u_0 :

$$\frac{m(t) - m_0}{A\psi\rho_w} = \int_0^\infty [u(t, x) - u_0] dx = \sum_{i=1}^n \int_{\lambda_i^* \sqrt{t}}^{\lambda_{i-1}^* \sqrt{t}} [u_i(t, x) - u_0] dx \quad (10)$$

Here $m(t)$ denotes the total mass of moisture in the absorbing sample (kg) at the time t (s), m_0 the initial mass of moisture (kg), A the absorbing surface (m^2), ψ the porosity (-) and ρ_w the density of water (kg/m^3).

Note that the term $(m(t) - m_0)/(A\psi\rho_w)$, on the left-hand side of Eq. (10), can be empirically determined by weighing the moist sample during the absorption process. Moreover, as demonstrated in Ref. [4], the right hand side of Eq. (10) can be written as follows:

$$\begin{aligned} & \int_{\lambda_i^* \sqrt{t}}^{\lambda_{i-1}^* \sqrt{t}} [u_i(t, x) - u_0] dx \\ &= \sqrt{\frac{4tD_i}{\pi}} \frac{(u_{i-1}^* - u_i^*) \left[e^{-\lambda_{i-1}^{*2}/(4D_i)} - e^{-\lambda_i^{*2}/(4D_i)} \right]}{\left[\text{erf}\left(\frac{\lambda_{i-1}^*}{\sqrt{4D_i}}\right) - \text{erf}\left(\frac{\lambda_i^*}{\sqrt{4D_i}}\right) \right]} \\ &+ \sqrt{t} [\lambda_{i-1}^* (u_{i-1}^* - u_0) - \lambda_i^* (u_i^* - u_0)] \end{aligned} \quad (11)$$

In order to characterize the whole diffusivity function, a series of n water uptake tests, having different initial water contents, is required. The parameters D_i are determined starting from the highest water content level and decreasing step by step to the lowest one. The first test is hence performed with initial water content $u_0 = u_{n-1}^*$, to determine the diffusivity of the nearly-saturated region D_n . Accordingly, Eq. (11) is written as follows:

$$\frac{m(t)-m_0}{A\psi\rho_w} = (1 - u_{n-1}^*) \sqrt{\frac{4tD_n}{\pi}} \quad (12)$$

from which we immediately obtain:

$$D_n = \left[\frac{m(t)-m_0}{A\psi\rho_w(1 - u_{n-1}^*)} \right]^2 \quad (13)$$

Each parameter $D_{k < n}$ can hence be determined through a test performed with $u_0 = u_{k-1}$, if the diffusivity values at higher water content $D_{i > k}$ are already known. To this aim, the function f is introduced:

$$f(\lambda_k, \dots, \lambda_i, \dots, \lambda_{n-1}, D_k) = \left| \frac{m(t)-m_0}{A\psi\rho_w} - \sum_{i=k}^n \int_{\lambda_i^* \sqrt{t}}^{\lambda_{i-1}^* \sqrt{t}} [u_i(t, x) - u_0] dx \right| + \sum_{i=k}^{n-1} |a_i - b_i| \quad (14)$$

in which $\lambda_{k-1} = \infty$. The coefficients a_i and b_i are given by Eqs. (15) and (16), according to Ref. [4]:

$$a_i = \sqrt{\frac{D_i}{\pi}} \frac{(u_{i-1}^* - u_i^*) e^{-\lambda_i^{*2}/(4D_i)}}{\left[\operatorname{erf}\left(\frac{\lambda_{i-1}^*}{\sqrt{4D_i}}\right) - \operatorname{erf}\left(\frac{\lambda_i^*}{\sqrt{4D_i}}\right) \right]} \quad (15)$$

$$b_i = \sqrt{\frac{D_{i+1}}{\pi}} \frac{(u_i^* - u_{i+1}^*) e^{-\lambda_i^{*2}/(4D_{i+1})}}{\left[\operatorname{erf}\left(\frac{\lambda_i^*}{\sqrt{4D_{i+1}}}\right) - \operatorname{erf}\left(\frac{\lambda_{i+1}^*}{\sqrt{4D_{i+1}}}\right) \right]} \quad (16)$$

The unknown parameters in Eq. (14) λ_i and D_k can be determined by searching for the zero of the function f through any suitable optimization technique. In this study, the matlab function “fminsearch”, based on the algorithm described in [5], has been used.

Note that the choice of the limit water contents u_i is arbitrary. If no information on the material behaviour is available, an equally spaced distribution can be used. On the other hand, a finer partition at high water content might be advantageous, in case a nearly exponential behaviour is expected. Obviously, the more tests are performed, the better the real diffusivity function can be approximated.

3 Experimental results

In this section, the method described above is tested by using five samples of calcium silicate insulation, whose properties are reported in Table 1. For the considered material, the capillary moisture content (i.e. reached at the end of the capillary absorption [6]) is similar to the moisture content determined through vacuum-saturation of the samples ($u_{cap} \approx 1$).

Table 1. Properties of calcium silicate.

Property	Symbol / expression	Dimension	Value
Density of the dry material	ρ_{dry}	Kg/m ³	333
Open porosity	ψ	-	0.852
Capillary moisture content	$\rho_w \psi u_{cap}$	Kg/m ³	850
Absorption coefficient	A_w	Kg/(m ² s ^{0.5})	0.7

The diffusivity function is approximated with $n=3$ steps, hence three water uptake experiments are necessary. The first absorption experiment has been performed with nearly dry samples, having an initial water content $u^*_0 \approx 0.07$. After the capillary moisture content is reached, the samples have been partially dried to the water content $u^*_1 \approx 0.75$, which represents the initial water content for the second absorption. Note that the moisture distribution in the sample after partial drying can be considered as nearly uniform, as shown in [7], due to the high moisture diffusivity of calcium silicate. The drying and absorption sequence is repeated one last time with $u^*_2 \approx 0.89$.

The moisture mass in the samples during the absorption is reported in Fig. 2 (a). It can be observed that the moisture mass increases almost linearly with the square root of the time until the so-called capillary saturation is reached ($u=1$). This linear behaviour confirms that the diffusion equation Eq. (1) can adequately describe the absorption process. In Fig. 2 (b) the obtained diffusivity function is compared with the results by Ref. [8]. A fair agreement can be observed.

In Fig. 3 (a) the limit of the dry region during the first absorption test ($u^*_0 \approx 0.07$) is shown at two different times. Note that the dry limit position corresponds to a single value of λ , according to Eq. (7). This value, reported in Fig. 3 (b) as a vertical continuous line, is in fair agreement with the curve $u(\lambda)$ described by Eq.(6) with the afore obtained diffusivity. Thus the above results are confirmed.

Fig. 2. (a) Mass of moisture in the five calcium silicate samples; (b) resulting diffusivity functions and results by another study (Ref. [8]). Sample dimensions: $0.1 \cdot 0.03 \cdot 0.1$ m, absorbing area: $3 \cdot 10^{-3} \text{ m}^2$, sample volume: $0.3 \cdot 10^{-3} \text{ m}^3$, dry sample mass: ≈ 100 g, capillary moisture content: ≈ 255 g.

Fig. 3. (a) Limit of the dry region at two different times during absorption; (b) curve $u(\lambda)$ and limit of the dry region (calcium silicate, sample 1).

4 Conclusions

A method is proposed to determine the diffusivity function of capillary active materials by means of water uptake tests. The method is based on an analytical approach, in which the diffusivity is approximated as a multiple step function of the water content. In this study, a first test has been performed by employing calcium silicate samples and by assuming a diffusivity function having three steps. The results are promising for a wider application of the method in the future. The application to other building materials, as well as the use of functions having more than three steps shall be investigated.

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