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Study of Moisture Transport by Numerical Modeling and Neutron Transmission Analysis

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Abstract

Moisture transport in porous building materials is described by a transport model that expresses the action of the several transport mechanisms of liquid water and water vapor in the porous system by a single material specific transfer coefficient. This parameter has to be determined by experimental measurement of moisture distributions inside samples exposed to known initial and boundary conditions. Neutron radiography is employed as experimental method because of its high sensitivity and good spatial resolution. The moisture distribution is determined from the raw data obtained in the measurement by a calculation procedure based on a signal transfer model of the neutron transmission. This approach is illustrated by two examples: the drying of a plain brick sample and the drying of a composite sample consisting of two brick elements separated by a layer of mortar.

Key Words: Porous materials, moisture transport, transfer coefficient, neutron transmission analysis, numerical modelling.

Untersuchung von Feuchtetransport mittels numerischer Modellierung und Neutronentransmissionsanalyse

Zusammenfassung

Der Feuchtetransport in porösen Baumaterialien wird durch ein Transportmodell beschrieben, wobei die verschiedenen Transportmechanismen von flüssigem Wasser und Wasserdampf in einem einzelnen materialspezifischen Transferkoeffi-

zienten zusammengefaßt werden. Dieser Parameter muß durch experimentele Bestimmung von Feuchteverteilungen in Proben, welche bekannten Anfangs- und Randbedingungen ausgesetzt werden, ermittelt werden. Als experimentelle Methode wird aufgrund ihrer hohen Empfindlichkeit und guten räumlichen Auflösung Neutronenradiographie eingesetzt. Die Feuchteverteilung wird aus den im Experiment gewonnenen Rohdaten mittels einer auf einem Signaltransfer-Modell der Neutronentransmission basierenden Auswerteprozedur bestimmt. Die geschilderte Vorgehensweise wird anhand zweier Beispiele illustriert: das Trocknen einer Probe aus Ziegelstein und das Trocknen einer aus einer Mörtelschicht zwischen zwei Ziegelstein-Elementen zusammengesetzten Probe.

Stichwörter: poröse Werkstoffe, Feuchtetransport, Transferkoeffizient, Neutronenradiographie, numerische Modellierung.

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1 Introduction

The movement of moisture inside building structures can cause important damage because the action of chemical contaminant agents transported by the water, the action of micro-organisms growing in the humid environment, the mechanical action of freezing and thawing or shrinkage and carbonation due to drying contribute to the degradation of the building substance. Therefore the understanding of moisture transport in building components is an important issue in building technology. As many building materials are porous, the theoretical modeling and experimental measurement of moisture transport in the porous system are important to the understanding of the transport processes. Furthermore, building components are usually composite structures consisting of elements made of different materials. Therefore an adequate description also has to take into account the interaction between different porous media.

This paper describes the general approach and then gives an overview of the analytical model and experimental technique. The applied methods are illustrated by two application examples describing the drying of a plain brick sample and of a composite sample consisting of a layer of mortar between two layers of brick.

2 General approach

The general approach is based on models of the object of study and the measurement process and on procedures derived from these models. It emphasizes the importance of modeling of both the mechanism that is studied and the measurement by which it is studied to achieve a correct interpretation. It consists of the following elements:

A. formulation/selection of a model of moisture transport in porous building materials in which the movement of moisture is determined by equations containing material-specific parameters;

B. application of the model from A to the description of moisture transport by numerical simulation of the process in building material samples of a given composition and geometry exposed to defined initial and boundary conditions;

C. experimental measurement of the moisture distribution at different times in building material samples of the same composition and geometry than those in B, exposed to the same initial and boundary conditions;

D. formulation of a model of the measurement process which describes the generation of the raw data obtained in the measurement;

E. application of the model from D to the formulation of an evaluation procedure which permits to extract the desired information, i.e. the shape of the moisture distribution, from the raw data.

When the procedure defined in E is applied to the raw data from C, the moisture distribution in the samples used in the experiment at the times of measurement is obtained and can be compared to the distribution at the corresponding times in the samples in the numerical model in B. The moisture transport parameters can then be determined by fitting the simulated profiles to the measured profiles by variation of the parameters from A. Fig. 1 gives a graphical representation of this approach.

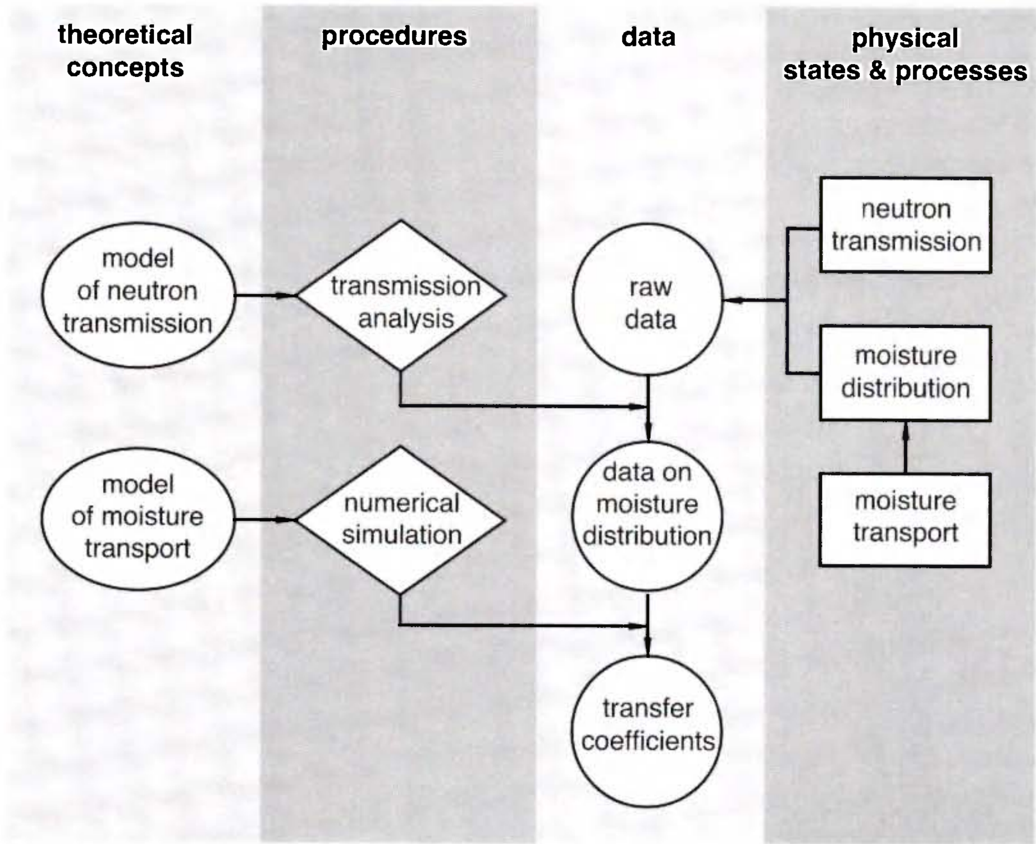

Fig. 1: Overview of general approach.

3 Transport model and numerical simulation

3.1 Physical description of the model

The size and the shape of pores present in a porous material exert a direct influence on the transport mechanism of water molecules. Despite the knowledge of the basic individual phenomena involved, like capillary transport, diffusion, surface diffusion, etc., it is not yet possible quantitatively to assess the influence of each of them on the global moisture transfer in a porous material such as concrete, mortar or brick. At the macroscopic level (i.e. in a representative finite volume of the porous structure), the aforementioned difficulty can be circumvented by defining a concentration-dependent transfer coefficient, which integrates all contributions of the different mechanisms to the global mass transfer. In this phenomenological description, the transient moisture flow can be described according to the Fick's law. If w represents the specific moisture content of the porous body (mass per unit of volume), the Fick's law is described by the following partial differential equation:

$$\frac{\partial w}{\partial t} = div(D_w(w) \cdot gradw) \tag{1}$$

in which is the moisture transfer coefficient depending on the actual moisture content D_w. Eq. (1) is used since at least two decades by many authors to describe in a realistic way the moisture transfer in porous building materials, such as cement-based materials [1-4] or brick [5]. Two cases will be considered here: either the whole sample consists of one material or it consists of several layers of different materials. The latter is a more complex case, but it applies in many situations under realistic conditions.

In this second case, the porous system consists of a juxtaposition of different porous materials, characterized by their own desorption isotherms and their moisture transfer coefficients. The materials may be in equilibrium with the same relative humidity, but with totally different moisture contents. In other words, the moisture content cannot anymore be used as potential to describe the flow process in a porous bi-material system. Instead, pore humidity h may be used as potential to overcome this problem. At a constant temperature, an infinitesimal variation of the pore humidity *(dh)* can be related to a corresponding infinitesimal variation of the moisture content *(dw)* by means of the desorption isotherm of the material :

$$dh = C(h) \cdot dw \tag{2}$$

in which $C(h)$ equals the co-tangent of the desorption isotherm curve $w(h)$, the inverse of this value represents the hygral capacity. In this way, the flow process can be described in terms of h by the following equation:

$$\frac{\partial h}{\partial t} = C(h) \cdot div(D_h(h) \cdot gradh) \tag{3}$$

The transfer parameters $D_w(w)$ and $D_h(h)$ are related by the following relationship:

$$D_h(h) = D_w(w) / C(h) \tag{4}$$

The formulations in terms of w (Eq. (1)) and h (Eq. (3)) are equivalent only if the temperature is constant and if the porous structure is not influenced by aging effects such as hydration in case of young mortar.

For simulating the drying process of the porous composite system, Eq. (3) must be solved conjointly with adequate boundary conditions and initial conditions. Above a critical value of the moisture content, it has been assumed that the loss of water of the system is governed by evaporation at the surface exposed to drying atmosphere. This means that the moisture flux J_s at the surface is given by :

$$J_s = A \cdot q \tag{5}$$

where A is the area of the exposed surface and q is the rate of evaporation, which can be roughly estimated from the measured moisture profiles.

At lower moisture content in the brick, the fixed potential boundary type is used, namely the humidity at the surface is the same as the external humidity:

$$h_s = h_{ext} \tag{6}$$

where h_s is the humidity at the exposed surface and h_{ext} the relative humidity of the surrounding atmosphere.

The chosen type of mixed boundary conditions used to describe our problem is based on the observation of the behavior of the measured moisture profiles at different drying times. In the numerical simulation, the moisture profile measured first (a few minutes after the start of the drying process) is assumed to be the initial moisture state of the system (converted in terms of humidity via desorption isotherms of the two materials in contact).

3.2 Numerical analysis

The finite volume method is used to numerically solve the problem. Eq. (1) and Eq. (3) are used in their integral formulation [6]. In a conveniently small finite element volume of the flow region, they can be written respectively as follows:

$$\frac{\partial}{\partial t}\int_V w dv = \int_V div(D(w) gradw) dv \tag{7}$$

$$\frac{\partial}{\partial t}\int_{\Delta V} h \cdot dv = \int_{\Delta V} C(h) \cdot div(D_h(h) \cdot gradh) \cdot dv \tag{8}$$

By means of the divergence theorem, the right-hand terms of Eq. (7) and Eq. (8) can be converted to a surface integral, and assuming average values of w and over , they can be rewritten respectively as:

$$V\frac{\partial w}{\partial t} = \int_\Gamma D(w) gradw \cdot dA \tag{9}$$

$$\Delta V \cdot \frac{\partial h}{\partial t} = \int_\Gamma C(h) \cdot D_h(h) \cdot gradh \cdot dA \tag{10}$$

The problem is then solved by the integrated finite difference method [6]: the flow domain is discretized into small subdomains, in which Eq. (9) and Eq. (10) can be approximated as linear equations. $D_w(w)$ and $D_h(h)$ are expressed as functions of a suitable form containing a number of parameters D_1, D_2, D_3... which are determined by comparing the calculated moisture profiles with the experimental data and looking for the best fit. This can be achieved by minimizing the quadratic error [4]. The form of the function $D_w(w)$ or $D_h(h)$ and the number of parameters depend on which general form provides the best fitting result. It can be expected that different forms and parameters will prove optimal for different building materials. Indeed, two different forms will be applied to the examples presented in this study.

It should be noted that the presented model and numerical technique deduce the transfer coefficients directly from the moisture profiles without having to consider the integral moisture loss.

4 Experimental measurement and evaluation of data

4.1 Measurement method

For the experimental determination of moisture profiles, a non-destructive technique sensitive to the presence of water and providing information on the spatial distribution of the moisture is required. Several suitable non-destructive-methods for measuring the moisture distribution inside a sample exist. They can be classified in two main groups: NMR methods [7] based on electromagnetic interaction with the water in the porous system and radiography methods based on weakening of radiation passing through matter, using X-rays [8], γ-rays [9] or neutrons [10] to visualize the contrast between regions containing different amounts of moisture. NMR methods can distinguish between free, physically bound and chemically bound water, but interference may be caused by the presence of paramagnetic ions in most building materials. Radiography methods do not differentiate between free and bound water, but are not subject to electromagnetic interference and may offer higher spatial resolution, depending on the neutron source quality [11]. Among the radiography methods, neutron radiography offers the highest hydrogen detection sensitivity.

Neutron radiography in general is based on the universal law of weakening of radiation passing through matter. It consist of a neutron source, a collimator functioning as a beam formatting assembly and of a plane position sensitive detector. The neutron beam penetrates the object and then reaches the detector which records the beam intensity at each point in the detector plane. This way, an image which is a projection of the object into the detector plane is obtained. In this study, the object is always a building material sample containing an unknown moisture distribution.

4.2 Evaluation procedure

For quantitative evaluation, the image is digitized into a grayscale pixel array, which can be described as a detector signal function $S(x,y)$, where (x,y) are coordinates in the detector plane and can only adopt the discrete values corresponding to the centers of the individual pixels. The numeric value $S(x,y)$ corresponding to a pixel centered at (x,y) depends on the neutron intensity that reached the detector plane in the area of that pixel, integrated over the exposure time and weighted with the response function of the detector. From this data, the humidity distribution in the sample has to be determined.

A model describing the radiography process as signal transfer and a suitable evaluation procedure have been formulated and applied to the study of moisture transport [12, 13]. The model describes the neutron beam as consisting of two components: *uncollided* neutrons which have penetrated through the sample without interacting and *collided* neutrons which have been scattered in the sample. Two situations are considered: a measurement with the detector is effectuated with and without a sample. The first measurement yields a digital image of the sample and the second yields a digital image of the empty beam profile, expressed respectively as detector signal functions $S(x,y)$ and $S_o(x,y)$. The signal $S(x,y)$ obtained in the measurement with sample is the sum of an uncollided component $S_u(x,y)$ and a collided component $S_c(x,y)$:

$$S(x,y) = S_u(x,y) + S_c(x,y) \tag{11}$$

Because of the influence of scattered neutrons, the first image cannot simply be normalized using the second as correction background. Instead, $S(x,y)$ is viewed as the result of a sum of signal transfer function applied to $S_o(x,y)$. The processes generating the uncollided and collided components are of a different nature and therefore are described by two different functions: an attenuation function $UNC(x,y)$ for the uncollided component and a point spread function $PSF(x,y,x',y')$ for the collided component [14]. $UNC(x,y)$ describes the attenuation of the beam in the sample at the coordinates (x,y) and $PSF(x,y,x',y')$ expresses the influence of scattering from a point at the coordinates (x',y') in the sample towards the point at the coordinates (x,y) in the detector plane:

$$S_u(x,y) = UNC(x,y) \cdot S_o(x,y) \tag{12}$$

$$S_c(x,y) = \int PSF(x,y,x',y')\, S_o(x',y')\, dx'\, dy' \tag{13}$$

By describing the signal $S(x,y)$ measured in the presence of the sample as result of signal transfer functions applied to the signal $S_o(x,y)$ in the absence of the sample, a simple and efficient procedure for the interpretation of the complex transmission process is obtained.

For a given material and geometry, a given neutron beam of known energy spectrum and a given detector with a known response function, *UNC* and *PSF* can be determined by Monte Carlo calculations. In this study, these calculations were carried out using the code MCNP 4A [15]. For any assumed moisture distribution $w_{hypothesis}(x,y)$, the detector signal $S_{hypothesis}(x,y)$ that would result can be calculated from $S_o(x,y)$ by applying *UNC* and *PSF*. The unknown actual moisture distribution $w(x,y)$ in the sample can be determined by several steps iterative steps by comparing the obtained $S_{hypothesis}(x,y)$ to the actual detector signal $S(x,y)$ and deriving a new assumption on the moisture distribution until $S_{hypothesis}(x,y)$ and $S(x,y)$ converge within the precision of measurement [13].

5. Examples

5.1 General remarks

In each of the two examples presented here, rectangular prismatic samples of dimensions 12 x 9 x 3 cm^3 are used. The samples are covered with adhesive Al-tape on all surfaces except one 12 x 3 cm^2 face to restrict moisture exchange with the environment to that surface. They are initially saturated with water and placed into an atmosphere of constant relative humidity at the time $t = 0$.

Then they are radiographed at suitable times to observe the drying. The measurements were performed at the neutron radiography station at the TRIGA Mark II reactor of the Atominstitute of the Austrian Universities [16], using a converter/film assembly type detector [17]. The raw data from the measurements is processed with the image analysis software Image Pro Plus , and the evaluation procedure is applied to obtain the moisture distributions at the times of measurement.

To determine the transfer coefficients, the integrated finite element method is applied as described in section 3. Because five faces of the sample are sealed, the flow is unidirectional and Eq. (9) and Eq. (10) are simplified to one-dimensional equations. As pointed out section 3., the transfer coefficients are deduced directly from the measured moisture profiles without using the integral loss of moisture to estimate them. Indeed it could be seen in a test of the latter method that by using transfer coefficients approximated from the integral moisture loss it was not possible to reproduce the measured profiles shown in the following examples.

5.2 Plain brick sample

The plain brick sample was exposed to an atmosphere of 64 % of relative humidity and radiographed at times $t = 1, 2, 7, 14$ and 21 days. Because the sample consists of only one material, Eq. (9) which explicitly contains the moisture w can be applied. When the sample is discretized into volume elements (i), Eq. (9) can be approximated as follows for each (i) exchanging moisture with its neighboring elements (i-1) and (i+1):

$$V_i \frac{\Delta w_i}{\Delta t} = D_{i-1,i} \frac{w_i - w_{i-1}}{x_i - x_{i-1}} A + D_{i+1,i} \frac{w_i - w_{i+1}}{x_i - x_{i+1}} A \qquad (14)$$

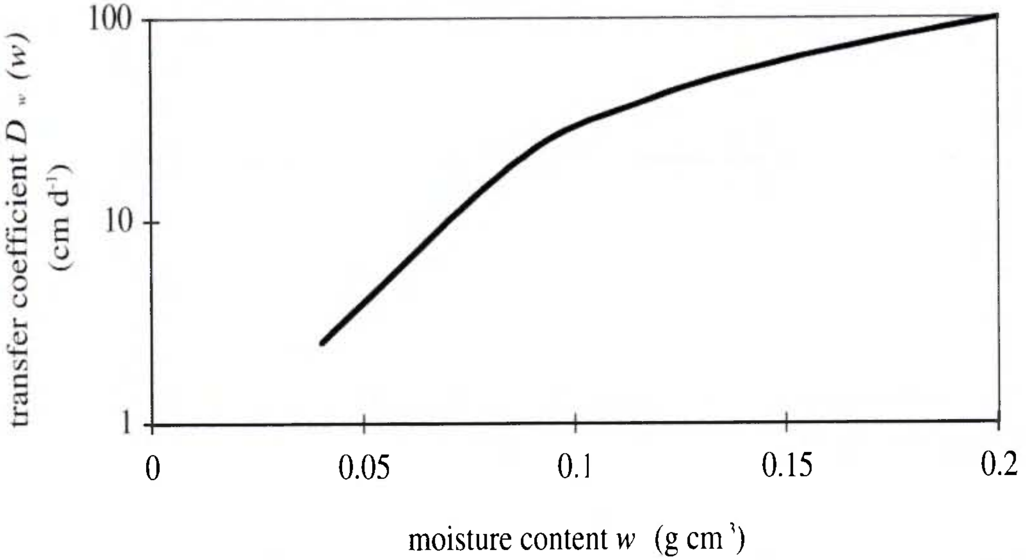

Fig. 2: Transfer coefficient $D_w(w)$ of the plain brick sample as a function of the moisture content *w*.

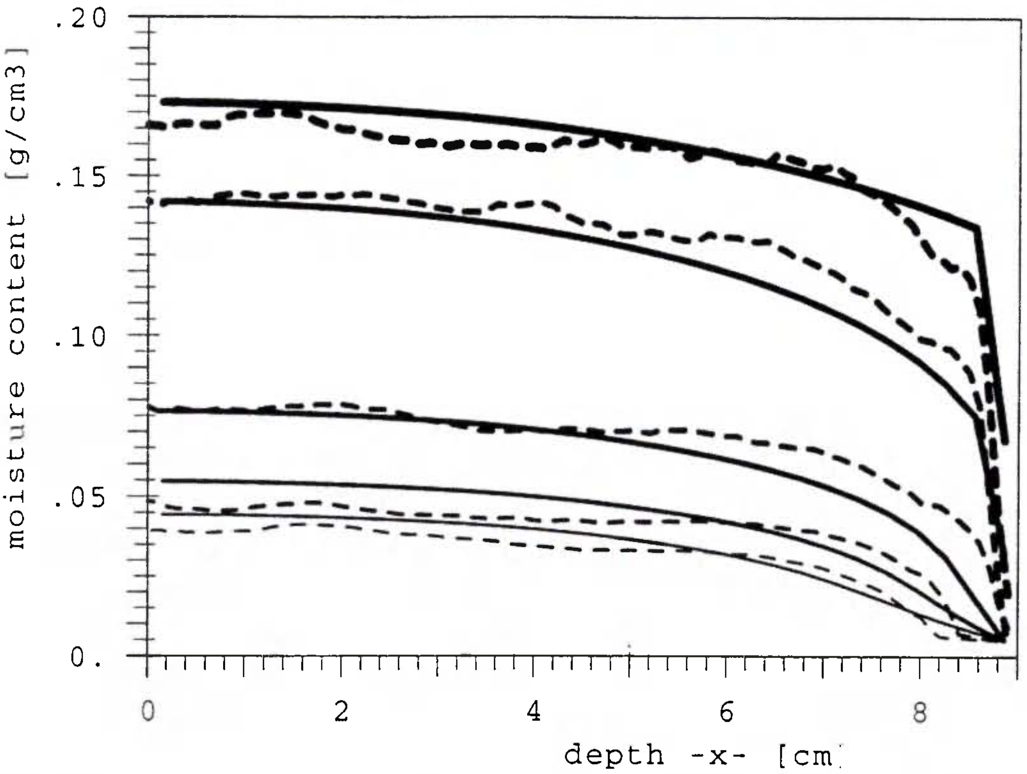

Fig. 3: Measured and calculated moisture profiles in the plain brick sample.

The terms $D^{k,l}$ are the harmonic mean values of the transfer coefficients of the adjacent elements (k) and (l). The boundary conditions are applied and a polynomial form of third order is assumed for $D_{..}(w)$:

$$D(w)=D_0+D_1w+D_2w^2+D_3w^3 \tag{15}$$

The resulting transfer coefficient as a function of w is displayed in Fig. 2 and a comparison of the measured and calculated profiles is shown in Fig. 3.

5.3 Composite brick/mortar sample

The sample consists of two layers of brick of dimensions 12 x 9 x 3 cm³ separated by a layer of mortar of dimensions 12 x 1 x 3 cm³ is determined in this example. The unsealed face of the sample is surface of one of the brick parts. The sample was radiographed at times t = 2, 8 16 and 21 days. Because the sample is composite, Eq. (10) is applied for the reasons given in section 3.1. For the i-th element of the discretized sample, it can be written as:

$$\Delta V_i \cdot \frac{\Delta h_i}{\Delta t} = C(h_i)\cdot A \cdot \left(D_h^{i-1,i} \cdot \frac{h_i - h_{i-1}}{x_i - x_{i-1}} + D_h^{i+1,i} \cdot \frac{h_i - h_{i+1}}{x_i - x_{i+1}}\right) \tag{16}$$

Again, the terms of Eq. (16) are the harmonic mean values of the transfer

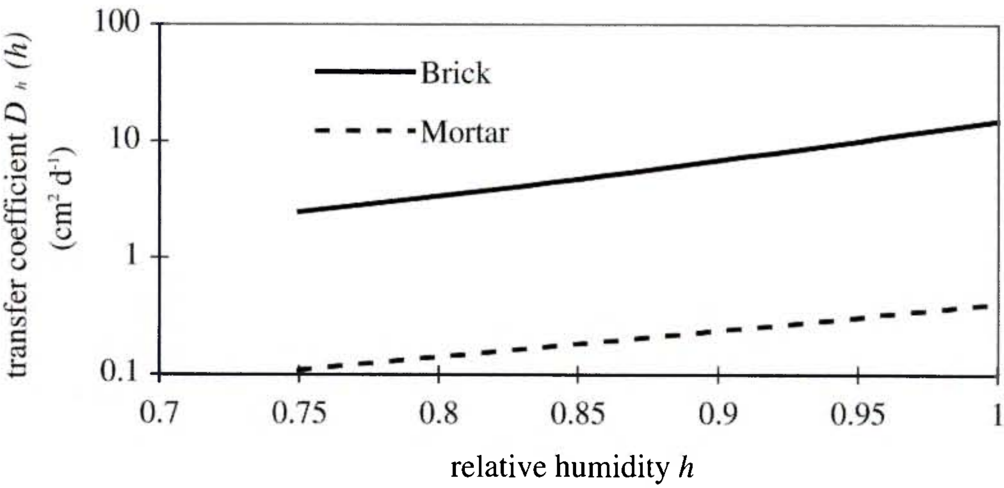

Fig. 4: Transfer coefficient $D_h(h)$ of brick and mortar in the composite sample as a function of the relative humidity h.

coefficients of the adjacent elements. The shape of the transfer coefficients of both materials is described by an exponential function:

$$D_h^k(h) = a_0^k + a_1^k \cdot \exp(a_2^k \cdot h) \tag{17}$$

where the index *m* stands for brick or mortar. The resulting functions $D_h(h)$ are presented in Fig. 4. In this numerical analysis, no special modeling is used to handle the interfacial zones between mortar and brick, but it can be seen in

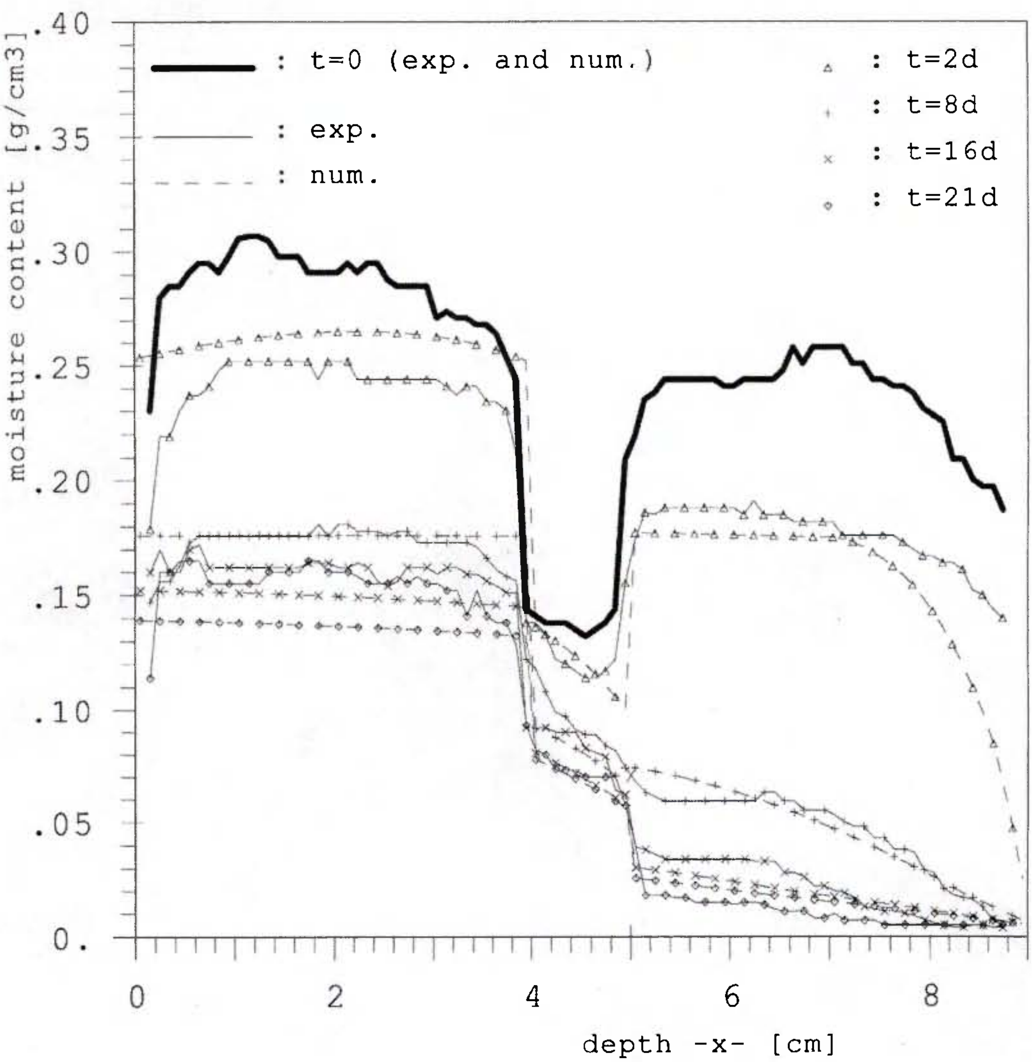

Fig. 5: Measured and calculated moisture profiles in the composite brick/mortar sample.

Fig. 5 that the calculated moisture profiles in these regions are quite satisfactory in comparison to the experimental ones. It must be outlined that in order to be consistent with the measured moisture profiles, a moisture loss through the left surface of the specimen was assumed in the calculation (this surface was not perfectly sealed, see Fig. 5).

6. Conclusion

The presented moisture transfer model and numerical technique have been applied successfully to two examples of different degrees of complexity. Neutron radiography has proved to be an efficient experimental tool because of its high moisture detection sensitivity and good spatial resolution. In combination with a suitable method of quantitative neutron transmission analysis it provides experimental data from which the parameters of the transfer coefficients can be determined. The method can be applied to the study of various mechanisms of moisture transport in components of many different porous building materials including composite structures.

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