

Modelling of coupled ion and moisture transport in porous building materials

T.Q. Nguyen^{a,b,*}, J. Petković^b, P. Dangla^b, V. Baroghel-Bouny^b

^a *Laboratoire Central des Ponts et Chaussées, Division for Concrete and Cement Composites, 58 Boulevard Lefebvre, F-75732 Paris, France*

^b *Université Paris-Est, Institut Navier, LMSGC, 2 allée Kepler 77420 Champs sur Marne, France*

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Abstract

In this paper, a physically based model describing the coupled ion and moisture transport is developed by combining existing theories of liquid water and water vapour transport with aqueous electrolyte theory. We derive the set of governing differential equations describing simultaneous movement of water in the vapour and liquid phases and consequent transport of ions in unsaturated porous media. The equations are developed in one-dimension, assuming isothermal conditions. It is also assumed that the movement of water in both the vapour and the liquid phases are first-order phenomena described by Fickian diffusion and Darcy's law, respectively. The influence of ions on liquid–vapour equilibrium is modelled here by considering the water activity term. The effect of salt crystallization on the transport properties is considered. The diffusion of the ions present in the system is modelled by solving the Nernst–Planck/local electroneutrality set of equations. A computer program has been developed to solve this highly non-linear problem. The validation of the model has been performed on the basis of a comparison between predicted kinetics of moisture or ion concentration profiles and measurement obtained by NMR on plaster/Bentheimer sandstone system during drying.

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1. Introduction

Moisture and in water soluble salts are notorious originators of structural deterioration, defacing by efflorescence and growth of all kinds of micro-organic matter when porous building materials are exposed to wetting–drying environment. Detailed information on the deterioration of construction and building materials can be derived from the fast amount of the literature (see, e.g. the prominent work and numerous publications of Binda et al. [1,2]).

The deterioration process determines maintenance needs and, finally, the service lifetime as elaborated by Bekker [3,4], see also the references therein. He initiated and

guided the work of Pel [5]. Bekker dealt with a life-cycle approach including economic consequences as well as the implications on scarce (natural and financial) resources. Furthermore, he formulated a logical relationship between deterioration and durability resulting in a clear and concise definition: durability is the resistance that follows from the inherent property or capacity to prevent decay. Dynamic moisture and ion transport is highly important topic in that respect.

In the building structures, plasters are often present as a finishing layer. The salt resistant plaster works either by accumulating the salts in the inner layer, where enough space should be provided for their crystallization, either by transporting of the salts to the surface of the plaster, where efflorescence occurs. But the performance of specially developed salt resistance plasters is not always as good as expected. In some cases salt crystallizes at the interface between two materials (masonry

* Corresponding author. Address: Laboratoire Central des Ponts et Chaussées, Division for Concrete and Cement Composites, 58 Boulevard Lefebvre, F-75732 Paris, France. Tel.: +33 140435301.

E-mail address: thai-quang.nguyen@lcpc.fr (T.Q. Nguyen).

and plaster), causing the plaster layer to detach. A better knowledge of the properties of the plaster (composition, physical properties and moisture transport behaviour) together with a sound awareness of the field situation (plaster/substrate combination, moisture and salt load, environmental conditions) may help in avoiding unsuccessful applications in practice. To understand these processes in more detail, we have investigated how transport and accumulation of salt in a plaster depends on the underlying masonry material. The object of this paper is to model the moisture and ion transport in the plaster/substrate system.

In fact, salt transport can be subdivided at least into two processes based totally on different mechanisms. Ions of dissolved salts can be transported with the migrating water by advection. The second transport mechanism is the ion diffusion driven by a concentration gradient. In addition, the previous experimental researches [6–9] show that the presence of salt strongly influences the kinetics of drying of water-containing porous media and lead to a reduction in the drying rate. Furthermore, the crystallization near the surface reduces the effective surface area available for the evaporation, leading to a decrease of the drying rate. Then, the coupled transport of moisture and ions involves complex chemical and physical model. Here, in the first part of this paper, the theoretical model is presented. It deals with the analysis and simulation of coupled ion and moisture transport in layered porous building materials taking into account insoluble salt precipitation. A physically based model describing these phenomena is developed by combining existing theories of liquid water and water vapour transport with aqueous electrolyte theory. We derive the set of governing differential equations describing simultaneous movement of water in the vapour and liquid phases and consequent transport of ions in unsaturated porous media. The equations are developed in one-dimension, assuming isothermal conditions. It is also assumed that the movement of water in both the vapour and the liquid phases are first-order phenomena described by Fickian diffusion and Darcy's law, respectively. The diffusion of the ions present in the system is modelled by solving the Nernst–Planck/local electroneutrality set of equations. The mass balance principles obtained for the different elements are supplemented with constitutive assumptions making the system of equations complete. The finite volume method has been used to discretize the coupled ion–moisture transport equations. A computer program has been developed to solve this highly non-linear problem. Then, results of an experimental test (moisture and sodium profiles), which have been measured non-destructively with a nuclear magnetic resonance (NMR) technique during drying of the plaster/Bentheimer sandstone system, were selected as a benchmark to test the computer program developed using the methodology described above, showing an excellent agreement between the numerical and the experimental results.

2. Governing equations of transport and mass balance equations

In this section a model is proposed that accounts for the isothermal drying process. The basic laws that describe the porous medium with simultaneous movement of fluid and ions through it will be presented. It is assumed that the mean velocity of the solid phase is zero; that is, no deformation of the solid phase is taken into account.

The transport of the liquid–ion mixture and that of the gas (mixture of water vapour and dry air) is assumed to be governed by the extended Darcy's law, which reads ($\alpha = l$ or g , for liquid and gas, respectively) for an isotropic porous medium:

$$v_{\alpha} = -\frac{K}{\eta_{\alpha}} k_{r\alpha}(S_l) \text{grad } p_{\alpha} \quad (1)$$

In Eq. (1), K is the permeability of the porous material (in m^2), which is an intrinsic property of the solid matrix and independent of the specific fluid characteristics. S_l is the liquid saturation rate. v_{α} , p_{α} , η_{α} and $k_{r\alpha}(S_l)$ are, respectively, the Darcy filtration velocity (in m s^{-1}), the pressure (in Pa), the dynamic viscosity (in Pa s) and the relative permeability associated with fluid α .

The relative permeabilities to liquid and to gas, which account for the variation of saturation degree due to moisture transfer, are usually approached using Mualem's model and Van Genuchten relationship [10]

$$k_{rl}(S_l) = S_l^{\xi} \left[1 - \left(1 - S_l^{1/m} \right)^m \right]^2 \quad \text{and} \\ k_{rg}(S_l) = (1 - S_l)^p \left[1 - S_l^{1/m} \right]^{2m} \quad (2)$$

where ξ and p are fitting parameters. The best value for the soils corresponds to $\xi = p = 0.5$ [5]. Using these expressions and the value of parameter m , which is derived from non-linear curve fitting of the capillary pressure curve (see Eq. (17)), the relative permeabilities to water and gas for the analysed material are calculated and presented in Fig. 1.

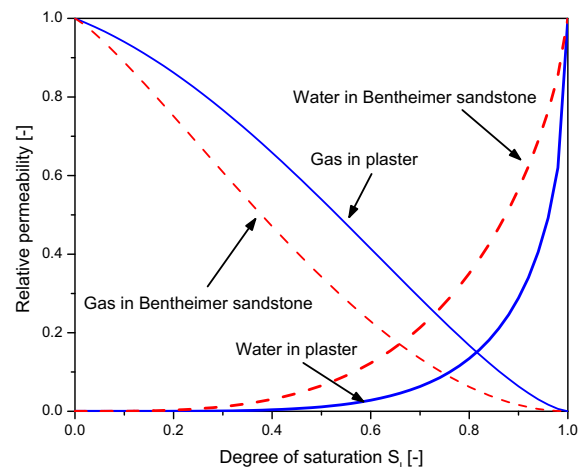


Fig. 1. Relative permeabilities to liquid water and to gas versus degree of saturation.

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