

COUPLED WATER AND CHLORIDE TRANSPORT IN CALCIUM SILICATE: PARAMETER IDENTIFICATION

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Abstract

Coupled water and chloride transport in calcium silicate is investigated in the paper. In the experimental part, the 1M-NaCl solution penetration into dry specimen is studied. Measured salt and moisture profiles are used for identification of parameters driving the salt solution transport through the porous structure of the material using inverse analysis. In the inverse analysis, the Bear's and Bachmat's diffusion-advection model is employed for the description of coupled water and salt transport. The salt diffusion coefficient as function of concentration and moisture diffusivity as function of moisture content are obtained.

Key words: water transport, chloride transport, calcium silicate

1 Introduction

The inverse mathematical analysis of experimentally determined salt concentration profiles depends on the assumed mode of salt transport in the porous material. Pursuant to previous experience with modeling of coupled moisture and salt transport, it can be concluded not only the diffusion mode of salt solution transport should be assumed [1]. Therefore, the mechanism of salt solution transport in this work is described by Bear and Bachmat diffusion-advection model [2] taking into account (in addition to salt diffusion in the liquid phase) the influence of moisture flow on salt transport and also the effect of bonded salt on pore walls. The salt mass balance can be expressed by relation (1)

$$\frac{\partial(wC_f)}{\partial t} = \text{div}(wD \text{grad}C_f) - \text{div}(C_f \vec{v}) - \frac{\partial C_b}{\partial t}, \quad (1)$$

where C_f is the concentration of free salts in water [kg/m^3], C_b the concentration of bonded salts in the whole porous body, [kg/m^3], D the salt diffusion coefficient, [m^2/s], \vec{v} the Darcy's velocity [m/s], and w the volumetric moisture content [m^3/m^3].

The water mass balance is expressed in formula (2),

$$\frac{\partial w}{\partial t} = \text{div}(\kappa \text{grad}w), \quad (2)$$

where κ is the moisture diffusivity [m^2/s].

Expressing Darcy's velocity in terms of moisture diffusivity,

$$\vec{v} = -\kappa \text{ grad}w, \quad (3)$$

the salt solution transport can be described by a system of two parabolic partially coupled differential equations with two principal material parameters, D and κ , and three input variables, C_f , C_b , w that must be determined experimentally.

2 Material and samples

In the experimental work, samples prepared from calcium silicate plates delivered by Calsitherm, Inc., Germany, were used. Calcium silicate plate was a low-density ($\rho = 230 \text{ kg/m}^3$) board product mainly used as capillary active inside insulation, because of its very high capillary absorption coefficient and capillary moisture content. The raw materials were calcium oxide and silica, which reacted with water to form calcium silicates. During the autoclaving process at high temperatures (due to the high pressure induced) air replaced water in the pores, so that fine porous structure was formed. Finally the product was dried. For the realization of suction experiments, the samples with dimensions 20 x 40 x 160 mm were used. These were dried in vacuum drier at temperature 80°C and all their lateral sides were water and vapor-proof insulated by an epoxy varnish. The samples for ion binding isotherm measurement had the dimensions of 40 x 40 x 10 mm.

3 Experimental methods

The arrangement of the experiment for determination of salt concentration profiles and water suction curves was analogous to standard water suction experiments. The samples were exposed by their 40 x 20 mm face to the penetrating 1M-NaCl solution. Duration of the experiment was 30, 60 and 90 minutes for three different groups of samples. After this time, the samples were cut into 8 pieces and in each piece water content and chloride concentration were measured. Moisture content was determined by the gravimetric method using weighing the moist and dried specimens. In the determination of chloride concentration, the particular samples were after drying first ground by a vibration mill so that grains smaller than 0.063 mm were obtained. Then the ground samples were overflowed by 80°C warm distilled water and leached. The samples were then left in constant climatic conditions of laboratory for two months and after that, the salt contents in particular leaches were determined using the ion selective electrode.

The ion binding isotherm of NaCl was determined according to the modified Tang and Nilsson adsorption method from [3]. The concentration of the solution varied in the range from 0.01 M to 1 M. Measurement of chlorides concentration was done using the pH/ION 340i device with utilization of ion selective electrode. On the basis of measured ion binding isotherm of NaCl, the function $C_b(C_f)$ was found and the profiles of bound and free chlorides were determined.

4 Method of inverse analysis

If we assume for simplicity 1-D salt solution transport, the equations (1) and (2), taking (3) into account, can be written as follows

$$\frac{\partial(wC_f)}{\partial t} = \frac{\partial}{\partial x} \left(wD \frac{\partial C_f}{\partial x} \right) + \frac{\partial}{\partial x} \left(C_f \kappa \frac{\partial w}{\partial x} \right) - \frac{\partial C_b}{\partial t}, \quad (4)$$

$$\frac{\partial w}{\partial t} = \frac{\partial}{\partial x} \left(\kappa \frac{\partial w}{\partial x} \right). \quad (5)$$

Then, the system of two parabolic equations can be subjected to an inverse analysis in a similar way as for one parabolic equation, provided the initial and boundary conditions are simple enough, and the material parameters D and κ can be identified as functions of water content and salt concentration.

The simplest possibility of such an inverse analysis is an extension of the Boltzmann-Matano treatment under the same assumptions of constant initial conditions and Dirichlet boundary conditions on both ends of the specimen for both moisture content and salt concentration where one of the Dirichlet boundary conditions is equal to the initial condition.

The Boltzmann transformation then leads to the system of equations

$$2 \frac{d}{d\eta} \left(C_f \kappa \frac{dw}{d\eta} \right) + 2 \frac{d}{d\eta} \left(Dw \frac{dC_f}{d\eta} \right) + \eta \frac{d(wC_f)}{d\eta} + \eta \frac{dC_b}{dC_f} \frac{dC_f}{d\eta} = 0, \quad (6)$$

$$2 \frac{d}{d\eta} \left(\kappa \frac{dw}{d\eta} \right) + \eta \frac{dw}{d\eta} = 0. \quad (7)$$

Performing the second transformation providing that in the known time $t = t_0$, $w(x, t_0)$, $C_f(x, t_0)$ and $C_b(x, t_0)$ are known,

$$z = \eta \cdot \sqrt{t_0}, \quad (8)$$

we have

$$2 \frac{d}{dz} \left(wC_f \kappa \frac{dw}{dz} \right) + 2 \frac{d}{dz} \left(Dw \frac{dC_f}{dz} \right) + \frac{z}{t_0} \cdot \frac{d(wC_f)}{dz} + \frac{z}{t_0} \cdot \frac{dC_b}{dC_f} \cdot \frac{dC_f}{dz} = 0 \quad (9)$$

$$2 \frac{d}{dz} \left(\kappa(z) \frac{dw}{dz} \right) + \frac{z}{t_0} \frac{dw}{dz} = 0. \quad (10)$$

From equation (10) we can determine

$$\kappa(z_0) = \frac{1}{2t_0 \left(\frac{dw}{dz} \right)_{z_0}} \int_{z_0}^{\infty} z \frac{dw}{dz} dz, \quad (11)$$

where $\kappa(z_0) = \kappa(w_0, C_{f0})$, $w_0 = w(z_0, t_0)$, $C_{f0} = C_f(z_0, t_0)$.

The analysis of equation (9) leads to the following formula for calculation of salt diffusion coefficient

$$D(z_0) = - \frac{C_f(z_0) \kappa(z_0) \left(\frac{dw}{dz} \right)_{z_0}}{w(z_0) \left(\frac{dC_f}{dz} \right)_{z_0}} + \frac{1}{2t_0 \cdot w(z_0) \cdot \left(\frac{dC_f}{dz} \right)_{z_0}} \int_{z_0}^{\infty} z \left(\frac{d(wC_f)}{dz} + \frac{dC_b}{dC_f} \frac{dC_f}{dz} \right) dz, \quad (12)$$

where $D(z_0) = D(w_0, C_{f0})$ and the value of $\kappa(z_0) = \kappa(w_0, C_{f0})$, is obtained from equation (11).

5 Results of inverse analysis and discussion

The measured moisture and salt concentration profiles and the ion binding isotherm of NaCl in calcium silicate are presented in Figures 1 – 3.

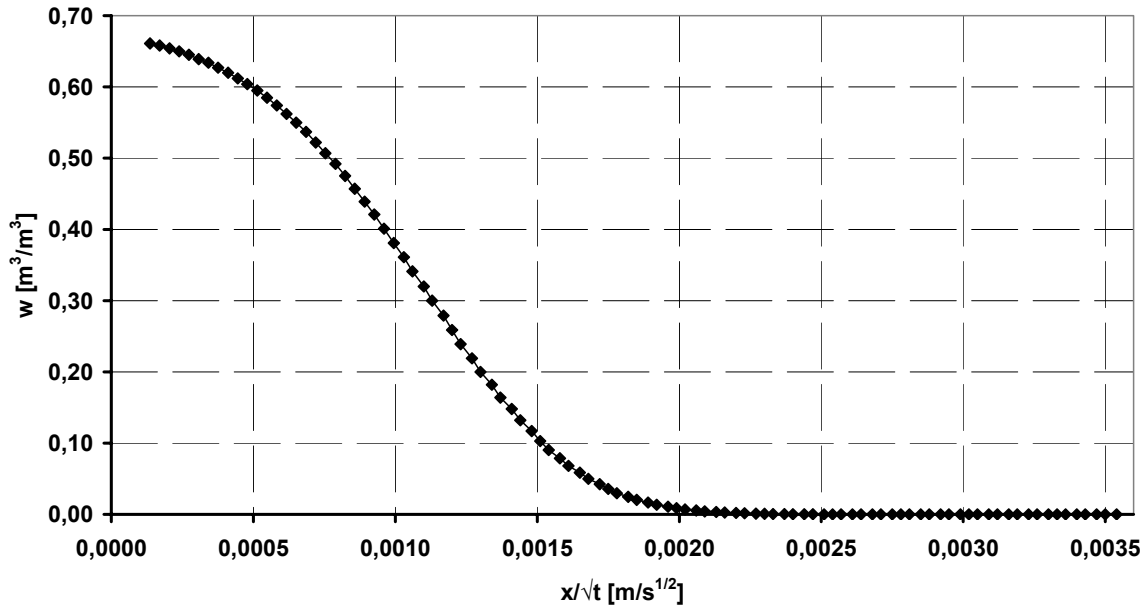


Fig. 1 Moisture profiles in Boltzmann form determined for 1M-NaCl solution penetration

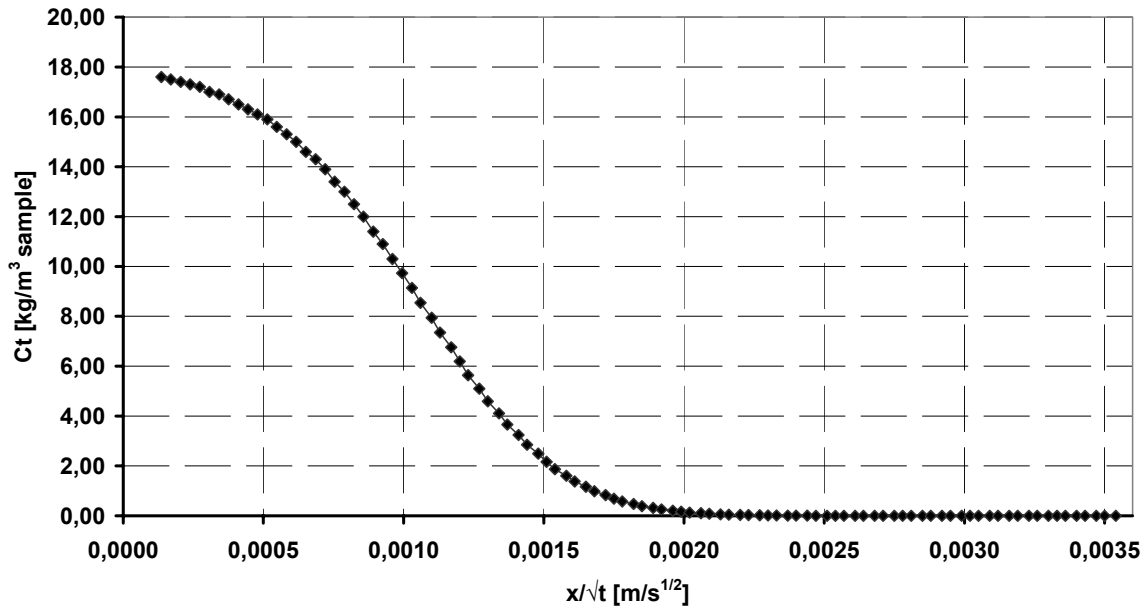


Fig. 2 Salt concentration profiles (total salt concentration) in Boltzmann form

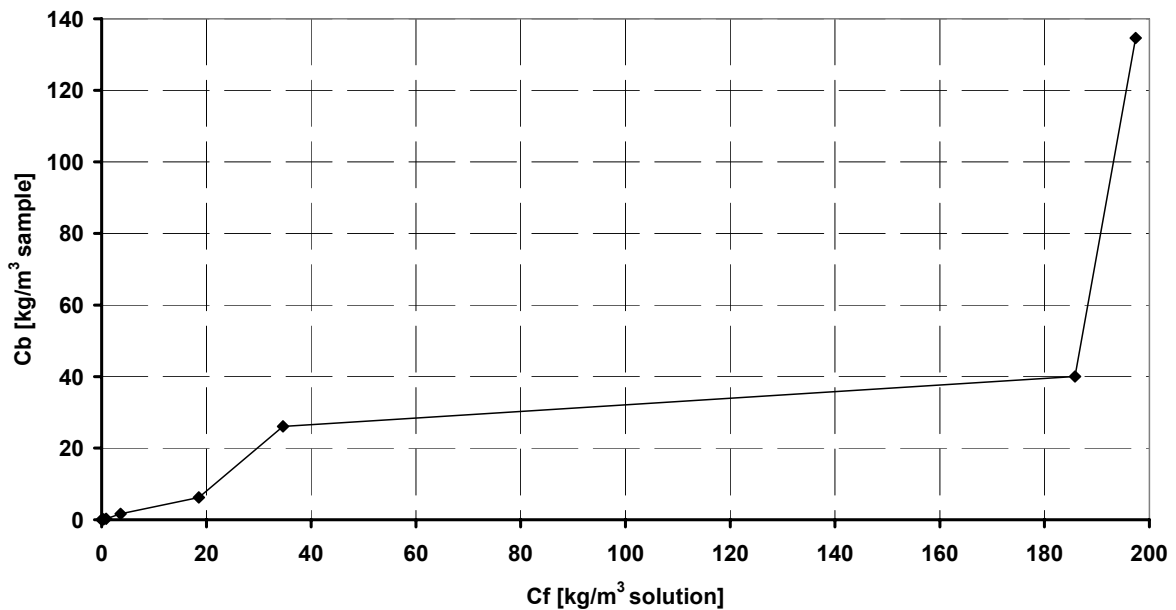


Fig. 3 Chlorides binding isotherm of calcium silicate

Fig. 4 shows the moisture diffusivity as function of moisture content calculated using the inverse analysis described before. We can see that obtained results correspond to the values typical for highly capillary active materials.

Fig. 5 shows the chloride diffusion coefficient in dependence on free ion concentration calculated using the $\kappa(w)$ function in Fig. 4. We can see that from the quantitative point of view, the calculated diffusion coefficient is quite high, about two orders of magnitude higher than the diffusion coefficients of most ions in free water. Therefore, the common diffusion mechanism was probably not the only driving force for the chloride transport within the liquid

phase and some other driving forces were taking place here. The most straightforward explanation is that this acceleration of chloride movement may be attributed to dispersion effects of the ions in the liquid phase but further, more exact analysis should be done in this respect.

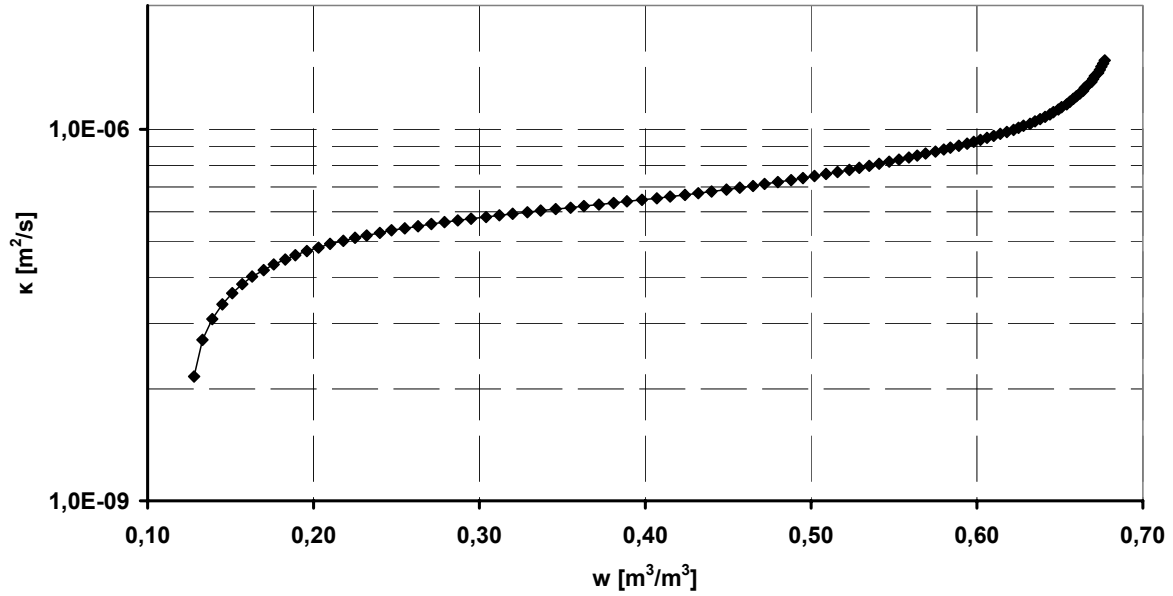


Fig. 4 Moisture diffusivity of calcium silicate as a function of moisture content calculated for 1M-NaCl solution penetration

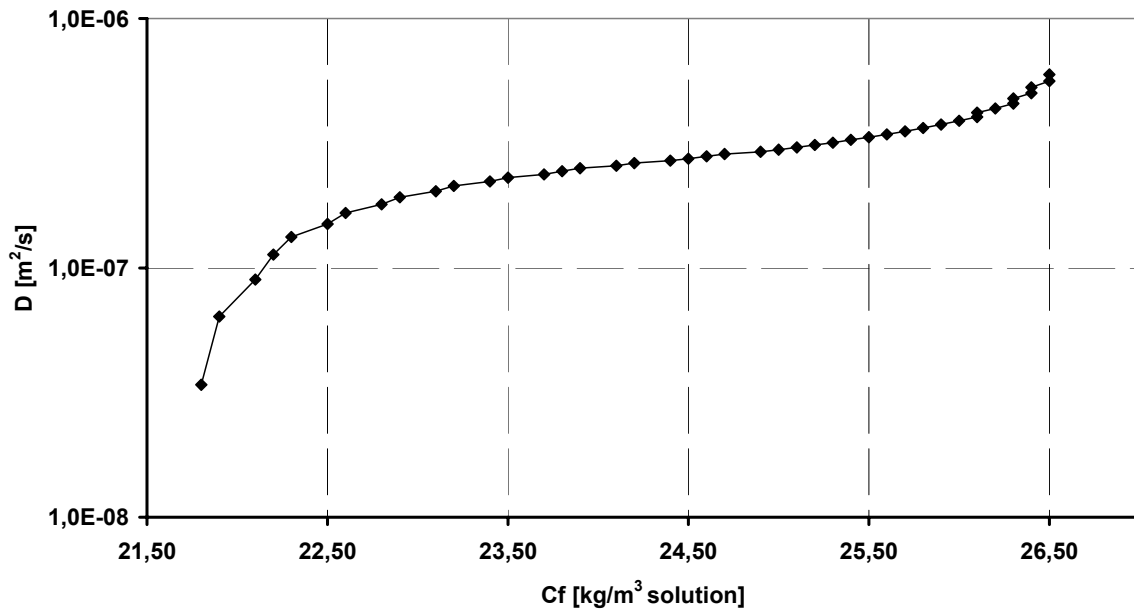


Fig. 5 Chloride diffusion coefficient of calcium silicate in dependence on concentration of free ions

6 Conclusions

The results presented in this paper contributed in certain extent to the explanation of the not yet very well explored problem of coupled moisture and salt transport in porous building materials. The obtained results revealed an interesting fact that the salt transport in the particular case of chloride penetration into calcium silicate analyzed in this paper was realized not only by diffusion and advection as it is commonly assumed but some other effects played an important role in the process as well, which speeded up the salt movement in the porous system. This acceleration of salt transport can be attributed most easily to dispersion effects of the salt in the liquid phase but it should be noted that this is a formal explanation only and an exact physico-chemical analysis is still needed.

Acknowledgement

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References

- [1] Pavlík Z, Jiříčková M, Černý R, Rovnaníková P 2004 Computational Analysis of the Parameters of Coupled Water and Chloride Transport in Cement Mortar on the Basis of Experimental Water and Chloride Profiles, *Cement Combinations for Durable Concrete*, Thomas Telford Publications, London, pp. 611-620.
- [2] Bear J, Bachmat Y 1990 Introduction to Modeling of Transport Phenomena in Porous Media, Vol. 4, Kluwer, Dordrecht.
- [3] Jiříčková M, Černý R 2004 Binding Isotherms of Different Types of Building Materials, *Proceedings of CIB W40 Meeting*, Glasgow Caledonian University, Vol. 1, 8.1 – 8.10.