

Mathematical modeling of water and salt transport in porous materials

R. Černý

*Department of Building Materials, Faculty of Civil Engineering,
Czech Technical University in Prague, Czech Republic*

Abstract

Most models applied in current research practice for the description of salt transport in porous materials are very simple. These employ Fick's diffusion equation for the salt concentration with a constant diffusion coefficient and constant initial and boundary conditions. Another extreme in this sense presents a consideration of fully coupled heat, moisture and chemical compound transport phenomena. A possible way out from the problems arising due to either oversimplification or too high complexity is to choose a reasonable compromise, i.e., a model that is somewhere in between these two extremes. Unfortunately, such models are still rarely used both in the research and technical practice. In this paper, a modification of the diffusion-advection model which takes into account not only the influence of water flow on salt transport but also the effect of salt bonding on pore walls is identified as the most promising for practical applications.

Keywords: water transport, salt transport, modelling, diffusion, advection, salt bonding.

1 Introduction

Porous materials applied in building structures often contain significant amount of various salts. They can originate from several sources. One of them is underground soil with water-soluble salts. In some building structures, particularly older buildings horizontal water-proof insulation is missing, so that salt solutions can be transported into materials of load bearing structures by capillary forces. Another source of salts in masonry is sodium and calcium chlorides used for winter maintenance of pavements and footways. They can



diffuse either into underground soil or directly into the masonry. Salts can also be formed by reactions of acid-forming gases in the air with basic components of building materials. Some salts can be formed by actions of living organisms and microorganisms. Water-soluble salts in the form of hydrated ions capable of transport in the porous system can also be presented in masonry materials themselves.

If salts are presented in porous system of masonry materials in the form of solution, they are mostly not dangerous. The harmful effects of such salts consist in the fact that after possible water evaporation salt crystals and crystal-hydrates are formed that often have crystallization pressures higher than the strength of the particular material. The pressure exerted on pore walls can then lead to material destruction.

The damage assessment of porous materials of building structures due to the effect of salts can be performed in simplest way by taking specimens from damaged walls and analyzing them in laboratory. This provides information on water content and on the type and amount of ions in material which is very useful for appreciation of the current state. The possible reasons for the presence of the particular ions can also be estimated on the basis of these analyses. However, it is very difficult to make reliable predictions of further damage on the basis of these data. This requires years or even decades of on site measurements, aside from the fact that the extent of such analyses is logically restricted by the amount of material which can be taken from a particular building.

Prediction of water and salt movement in the walls of building structures can be done effectively by means of mathematical and computational modeling. In this way, the time development of water and salt concentration fields can be obtained which is crucial for a proper assessment of possible future damage. However, the accuracy of simulated water and salt concentration fields critically depends on the availability of all input parameters.

There are two types of these parameters which have to be known in advance. The first are initial and boundary conditions. Initial conditions can be determined using on site analysis of water and salt concentration fields in the walls. Boundary conditions are of two types. The first of them are meteorological data for temperatures, relative humidities, rainfall and solar radiation, possibly also concentration of acid-forming gases in the atmosphere. This type of data can be obtained from meteorologists in the form of so-called TRY (Test Reference Year) data which present certain average values over a sufficiently long time period. The second type of boundary conditions involves water content and salt concentration in the underground soil close to the studied building. These data can be obtained again by on site analysis.

The second type of input parameters are water and salt transport and storage parameters of the materials of the wall which appear in water and salt mass balance equations. These parameters can be determined by common laboratory methods. Samples for the determination of water and salt transport and storage parameters can be obtained most easily from the walls of the analyzed building. If this is not possible, samples of building materials can be obtained from the

original sources which are usually known for a particular building or, in worst case, similar materials available at the market can be used.

The type and amount of material parameters necessary as input parameters of computational models of water and salt transport depend primarily on the type of physical model which was chosen for the description of transport processes taking place in a material. This choice should be done taking into account two basic contradictory requirements. First, the model is supposed to describe all the principal phenomena related to the transport and storage of water and salt in the porous space with a sufficient accuracy, as omitting any principal effect would lead to a significant departure from the reality. On the other hand, the number of parameters which are to be obtained from the experiments should not be too high; it has to reflect the feasibility of the necessary experiments in reasonable time. Therefore, some compromises in the choice of the model are always to be done.

In this paper, an analysis of current models of water and salt transport in porous materials used in both scientific and technical practice is performed and perspective models having good potential for common practical applications are identified.

2 Basic diffusion model

The basic diffusion model of salt transport in porous materials is very simple, and employs 1-D Fick's diffusion equation for the salt concentration with constant diffusion coefficient and constant initial and boundary conditions,

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} \quad (1)$$

$$C(0, t) = C_0 \quad (2)$$

$$C(\infty, t) = 0 \quad (3)$$

$$C(x, 0) = 0, \quad (4)$$

where D is the diffusion coefficient, C the salt concentration, C_0 the salt concentration at the exposed boundary, x the distance from the exposed boundary, t the time.

The problem (1)–(4) has a very simple mathematical solution (e.g., [1]):

$$C(x, t) = C_0 \left[1 - \operatorname{erf} \left(\frac{x}{2\sqrt{Dt}} \right) \right]. \quad (5)$$

Therefore, the diffusion coefficient can be identified from the measured concentration profiles using very simple methods, for instance the common Newton iteration formula. This is certainly the main reason for the high application frequency of this model which was employed for instance by Tuutti [2], Funahashi [3], Cady and Weyers [4], Weyers [5], Zemajtis et al. [6], Costa and Appleton [7] and many others. Some of the authors, for example Zemajtis et al. [6], assumed the surface concentration as a function of the square root of time, or in more general form (e.g., Costa and Appleton [7]) as a power function of time,

$$C_0(t) = C_1 t^n, \quad (6)$$

where C_1 is the surface chloride concentration after one year, t is expressed in years, and n is an empirical coefficient.

The model (1)–(4), which can be considered as the simplest choice ever in modeling salt transport contains several serious flaws that have to be taken into account in any practical application of it. The main problems with the model consist in the assumption of constant diffusion coefficient and in the fact that it neglects the influence of water transport on the transport of salts. As a consequence, a single value of the diffusion coefficient can never be obtained from the analysis of measured concentration profiles, particularly if the measurements are performed over longer time periods. The diffusion coefficient then appears as a function of time and usually is assumed to have the form

$$D(t) = D_1 t^{-m} \quad (7)$$

where D_1 is the diffusion coefficient at one year, t is expressed in years and m is an empirical coefficient.

Nevertheless, this model proved to be useful in many practical applications because the calculated diffusion coefficients have at least a relative value, i.e., it is possible to compare diffusion coefficients in different types of materials and different environments.

3 Improved diffusion models

The simplest and most straightforward improvement to the description of salt transport in porous materials given in the previous Section is the replacement of the linear diffusion problem (1)–(4) by a nonlinear one which means an assumption of the diffusion coefficient to depend on the salt concentration. Eq. (1) can then be written as

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} \left(D(C) \frac{\partial C}{\partial x} \right) \quad (8)$$

However, this assumption leads to a necessity to apply some more sophisticated methods for the analysis of measured salt concentration profiles than using just the solution in the form (5). A classical Boltzmann-Matano analysis seems to be an appropriate first-choice solution to this problem (see, e.g., [8] for details).

Another possibility for the improvement of the classical diffusion model (1)–(4) consists in a formal inclusion of water transport into the salt transport problem using the concept of apparent transport parameters [9]. The main difference between the apparent parameters and the thermodynamically “pure” parameters of the coupled water and salt transport is that the apparent parameters do not express “pure” effects, but combined effects. So, the apparent salt diffusion coefficients include not only the free salt diffusion in the porous space but also for instance the effect of salts bonding on the pore walls and the effect of salt transport due to the water movement. The notion of apparent moisture diffusivity then means that it is related not to the water itself, but to the salt-in-water solution, i.e. the whole liquid phase.

Under these simplifying assumptions, the same parabolic differential equations and the same boundary and initial conditions for both water transport and salt transport can be formally obtained, namely

$$\frac{\partial C}{\partial t} = \text{div}(D(C) \text{grad } C) \quad (9)$$

$$C(0, t) = C_1 \quad (10)$$

$$C(\infty, t) = C_2 \quad (11)$$

$$C(x, 0) = C_2, \quad (12)$$

where C is either water concentration or chloride concentration, D is either the apparent moisture diffusivity or the apparent salt diffusion coefficient. Therefore, the calculation of concentration-dependent diffusion coefficients from the measured salt concentration profiles could be done using basically the same inverse methods as those for the determination of moisture-dependent moisture diffusivity or temperature-dependent thermal conductivity (see [8]).

The main flaw of this treatment is that the apparent parameters are in fact not any objectively defined physical quantities. So, the concept of apparent transport coefficients can be useful in the solution of a class of case studies only where the same initial and boundary conditions are valid. In other cases, it is useless.

4 Diffusion-advection models

Diffusion-advection models present further substantial improvement to the physical description of salt transport in porous materials. It consists mainly in taking the influence of moisture flow on the salt transport into account. Another effect usually considered in the diffusion-advection models (in addition to those appearing in diffusion-type models) is the salt bonding on the pore walls. This type of model of salt solution transport in porous media was probably first described by Bear and Bachmat [10] who expressed the salt mass balance by the relation

$$\frac{\partial(wC_f)}{\partial t} = \text{div}(wD \text{grad } C_f) - \text{div}(C_f \vec{v}) - \frac{\partial C_b}{\partial t} \quad (13)$$

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], w the volumetric moisture content [m^3/m^3], D the salt diffusion coefficient, [m^2/s], \vec{v} the Darcy's velocity [m/s],

$$\vec{v} = -k \text{grad } h \quad (14)$$

k is the hydraulic conductivity [m/s] and h the hydraulic head [m]. The water mass balance was in the model from [10] expressed as

$$\frac{\partial w}{\partial t} = -\text{div } \vec{v} \quad (15)$$

As follows from Eqs. (13)–(15), a convective (mechanistic) type of model of water transport which is common for instance in soil science was used in the Bear and Bachmat model [10]. This type of model is, however, not common in building physics where diffusion types of models of water transport are mostly preferred

(see, e.g., [8] for a detailed analysis). Therefore, Pel et al. [11] in modeling the transport of NaCl solution in calcium silicate brick modified the Bear and Bachmat diffusion-advection model [10] by expressing the Darcy's velocity in terms of moisture diffusivity κ [m²/s],

$$\vec{v} = -\kappa \text{grad} w, \quad (16)$$

and substituting it in Eqs. (13) and (15) instead of Eq. (14). Their final model had then the following form:

$$\frac{\partial(wC_f)}{\partial t} = \text{div}(wD \text{grad} C_f) + \text{div}(C_f \kappa \text{grad} w) - \frac{\partial C_b}{\partial t} \quad (17)$$

$$\frac{\partial w}{\partial t} = \text{div}(\kappa \text{grad} w). \quad (18)$$

The salt solution transport model (17), (18) presents a system of two parabolic partially coupled differential equations with two principal material parameters, D and κ , and three field variables, C_f , C_b , w . The third necessary equation to achieve a unique solution to the system of Eqs. (17), (18) is the ion binding isotherm $C_b = C_b(C_f)$ which is to be determined experimentally and then substituted in an analytical form in Eq. (17).

The principal problem with the determination of material parameters within the framework of the model (17), (18) consists in the fact that in Eq. (17) appear both D and κ . This leads to a necessity to solve together the inverse problems to both (17) and (18), in general. However, solving inverse problems of parabolic problems is not an easy task even in the case of one equation (see [8] for a more detailed analysis and a survey of methods). So, it is quite logical that most researchers try to avoid this problem.

One of the possibilities how to deal with the solution of the inverse problem for D and κ in coupled water and salt transport is to neglect D as it was done in [11]. However, this idea did not appear as particularly useful even in the original paper because after solving the inverse problem in this way and performing the subsequent forward analysis the agreement between the experimental and computational Na⁺ ions concentration profiles was not very good.

Another method was proposed in [12] where two simple experiments were assumed for the identification of moisture diffusivity and salt diffusion coefficient. In the first experiment, the moisture diffusivity κ was determined in common way using inverse analysis of moisture profiles measured during the penetration of distilled water into a dry sample. As a result, a $\kappa(w)$ function was obtained. In the second experiment, the salt solution of a chosen concentration penetrated into a water-saturated sample and the salt diffusion coefficient D was determined using inverse analysis of measured salt concentration profiles. In this way, a $D(C)$ function was determined.

However, neither the concept of D and κ identification presented in [12] can be considered a general solution of the problem (17), (18); its application has some limitations. First, it can be applied for dilute solutions only because otherwise the moisture diffusivity would also be function of salt concentration. Second, its application is limited to low-bonding salts for the particular material because the analysis does not include the ion-binding isotherm.



The first limitation is rather critical. For concentrated solutions it would not even be sufficient to measure moisture diffusivity as function of the concentration of penetrating solution in a series of the above experiments. Such moisture diffusivities could not be successfully applied in any general coupled water and salt transport problems as the salt concentration is mainly function of position.

On the other hand, the second limitation of the method would be relatively easy to cure. With the measured ion binding isotherm, $C_b = C_b(C_f)$, the salt diffusion coefficient in the second proposed experiment could be calculated using the solution of the inverse problem to the equation

$$\left(1 + \frac{1}{w_{sat}} \frac{\partial C_b}{\partial C_f}\right) \frac{\partial C_f}{\partial t} = \text{div}(D \text{ grad} C_f), \quad (19)$$

which is only slightly different from the solution of the problem (9)–(12).

All the above mentioned methods for the identification of the moisture diffusivity and salt diffusion coefficient from moisture and salt concentration profiles used simplifications leading to the solution of inverse problems to one parabolic equation in 1-D approximation which was a logical procedure because the unknown solution of a more complicated problem was converted to the solutions of simpler, well known problems in this way. This quite a standard treatment is, however, in the particular case of the system of Eqs. (17), (18) not absolutely necessary. Theoretically, the system of equations (17), (18) 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. The material parameters D and κ can then 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 (see [8] for details of the original procedure) under the same assumptions of 1-D approximation, 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

$$\eta = \frac{x}{\sqrt{t}} \quad (20)$$

then leads to the system of equations

$$2 \frac{d}{d\eta} \left(C_f \kappa \frac{dw}{d\eta} \right) + 2 \frac{d}{d\eta} \left(Dw \frac{dC_f}{d\eta} \right) + \eta \frac{d(wC_f)}{d\eta} + \eta \frac{dC_b}{dC_f} \frac{dC_f}{d\eta} = 0 \quad (21)$$

$$2 \frac{d}{d\eta} \left(\kappa \frac{dw}{d\eta} \right) + \eta \frac{dw}{d\eta} = 0. \quad (22)$$

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,

$$z = \eta \cdot \sqrt{t_0}, \quad (23)$$

we have

$$2 \frac{d}{dz} \left(w C_f \kappa \frac{dw}{dz} \right) + 2 \frac{d}{dz} \left(D w \frac{dC_f}{dz} \right) + \frac{z}{t_0} \cdot \frac{d(w C_f)}{dz} + \frac{z}{t_0} \cdot \frac{dC_b}{dC_f} \cdot \frac{dC_f}{dz} = 0 \quad (24)$$

$$2 \frac{d}{dz} \left(\kappa(z) \frac{dw}{dz} \right) + \frac{z}{t_0} \frac{dw}{dz} = 0. \quad (25)$$

From equation (25) we can determine

$$\kappa(z_0) = \frac{1}{2t_0 \left(\frac{dw}{dz} \right)_{z_0}} \int_{z_0}^{\infty} z \frac{dw}{dz} dz \quad (26)$$

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 (24) leads to the following formula for calculation of salt diffusion coefficient

$$\begin{aligned} D(z_0) = & - \frac{C_f(z_0) \kappa(z_0) \left(\frac{dw}{dz} \right)_{z_0}}{w(z_0) \left(\frac{dC_f}{dz} \right)_{z_0}} + \\ & + \frac{1}{2t_0 \cdot w(z_0) \cdot \left(\frac{dC_f}{dz} \right)_{z_0}} \int_{z_0}^{\infty} z \left(\frac{d(w C_f)}{dz} + \frac{dC_b}{dC_f} \frac{dC_f}{dz} \right) dz, \end{aligned} \quad (27)$$

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 (26).

5 Fully coupled models

Fully coupled heat, moisture and chemical compound transport models present another extreme to the simplest Fick's model (1)–(4), in describing salt transport in porous materials. Among the most advanced models of this type, the model by Grunewald [13] belongs to very promising (see, e.g., the comments in [8] for more details). From the theoretical point of view, this type of models presents an ideal solution to the problem of salt transport in porous materials because the description of transport phenomena in these models is definitely closer to the physical reality than in the case of diffusion or diffusion-advection models. However, the main problem with the fully coupled models consists just in their complexity and particularly in the fact that they require too many parameters to be determined in advance. The measurements of some of them are very time consuming so that for instance determination of liquid convection coefficients can take several months if static methods are used. In addition, all coefficients should be measured as functions of all state variables; this means at least a

dependence on temperature, moisture content and salt concentration. Therefore, fully coupled models can be reasonably used only in the case that a database of necessary material parameters is already available.

6 Conclusions

The analysis of models of salt transport in porous materials in this paper revealed that an application of both too simple and too complex models is in the current scientific and technical practice not very desirable. Oversimplified models, such as the linear diffusion model of salt transport assuming just the salt concentration gradient as the only driving force of salt transport, can lead to an unacceptable distortion of physical reality. On the other hand, very complex models can face almost irresolvable problems with the accuracy of input parameters which may lead to similar distortions, which are maybe even more dangerous than in the case of oversimplified models because many researchers tend to consider this type of models mainly from the point of view of their theoretical qualities. Therefore, a reasonable compromise between these two extremes seems to be necessary. Taking into account the current state of knowledge of the modeling of salt transport in porous materials and the feasibility of the experiments for the determination of input parameters of computational models, a modification of the diffusion-advection model which takes into account not only the influence of water flow on salt transport but also the effect of salt bonding on pore walls can be considered as the most promising for practical applications.

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