

Numerical modelling of salt, moisture and energy transport in porous media considering kinetics of salt phase changes

Marcin Koniorczyk and Dariusz Gawin

Department of Building Physics and Building Materials, Technical University of Łódź, Al. Politechniki 6, Łódź 90-924, Poland
e-mails: marcin.koniorczyk@p.lodz.pl, dariusz.gawin@p.lodz.pl

Abstract

One of the most adverse phenomena which are related to the salt and moisture presence in the pore system of building materials is salt crystallization. The process is associated with the solution supersaturation ratio. The salt phase change kinetics is taken into account during the modelling of coupled moisture, salt and heat transport. To solve the set of governing, differential equations the finite element and finite difference methods are used. Three different rate laws are assumed in the modelling the salt phase change. The drying, cooling and warming of cement mortar sample, during which the salt phase change occurs, have been simulated using the software developed. The changes of salt concentration in the pore solution and the amount of precipitated salt due to variation of boundary conditions are calculated and discussed. Results obtained in numerical simulation assuming the first, second and fourth order rate law indicate that the higher order of the rate law, the longer time delay between the change of boundary conditions and the salt precipitation.

Keywords: salt, moisture transport, kinetics, phase change

1. Introduction

Coupled transport of water and salt are widely recognized as major factor of porous materials damage. Correns and Steinborn [1] derived the equation for maximum stress caused by crystals growth, which is a function of the salt solution supersaturation, S :

$$\Pi^c = \frac{RT}{V_m} \ln S. \quad (1)$$

In order to predict and calculate the solution supersaturation one has to consider the kinetics of the salt phase change.

2. Mathematical model

The presented mathematical model is an extension of the one that describes the heat and moisture transport in deformable porous materials [2] considering additionally salt mass balance equation and its influence on the heat and moisture transport. A porous material consists of the following phases: solid skeleton, liquid water (salt solution), water vapour and precipitated (crystallized) salt. It is assumed that only one salt is dissolved in the solution. The voids in the skeleton are filled partly with a liquid phase consisting of water and dissolved salt, partly with a gaseous phase consisting of dry air and water vapour, and partly with the precipitated salt. The liquid content is described by the water saturation degree, S_w . Salt appears in two phases: the former is the salt dissolved in the liquid phase, described by the mass concentration, ω , the latter is the precipitated salt which is described by the degree of pore saturation with the precipitated salt, S_p . The degrees of saturation with the all phases of the material follow the formula: $S_g + S_w + S_p = 1$. It is assumed that the solution is ideal and the gas is perfect gas. The chosen primary variables of the model are: $p^g(\mathbf{x}, t)$, $p^c(\mathbf{x}, t)$, $T(\mathbf{x}, t)$, $\omega(\mathbf{x}, t)$ and $\mathbf{u}(\mathbf{x}, t)$, and $S_p(\mathbf{x}, t)$ is internal variable of the model.

The mathematical model consists of five governing equations: water mass conservation, dry air mass conservation, salt mass conservation, energy conservation and linear

momentum conservation as well as evolution equation describing salt precipitation / dissolution kinetics.

2.1. Governing equations

Using Volume Averaging Theorem five macroscopic balance equations were derived. At the macroscopic scale one can measure all the necessary coefficients and material properties (density of materials, water dynamic viscosity, permeability, diffusivity factors, characteristic lengths of dispersion) experimentally. Because of the lack of available space only two of the governing equations will be presented in the extended abstract. It is assumed that salt influences the water density, dynamic viscosity and water retention characteristic [3]. The sources or sinks of dissolved salt influence the saturation degrees of water and gas due to the physical constraint, $S_g + S_w + S_p = 1$. The mass conservation of the salt dissolved in the fluid phase and precipitated (crystallized) salt is expressed as:

$$\begin{aligned} & \phi \frac{\partial}{\partial t} (\rho^w \omega S_w) - S_w \omega \rho^w \beta_s (1 - \phi) \frac{\partial T}{\partial t} + \phi \rho^p \frac{\partial S_p}{\partial t} + \\ & + S_w \omega \rho^w \operatorname{div} \left(\frac{\partial \mathbf{u}}{\partial t} \right) + \operatorname{div} (\phi S_w \omega \rho^w \mathbf{v}^{ws}) + \operatorname{div} (\mathbf{J}^{dysp}) = 0 \end{aligned} \quad (2)$$

The enthalpy conservation equation of the multiphase medium, obtained by summing the appropriate balance equations of the constituents includes the heat effects due to phase change of water and heat released during the salt precipitation process (the terms on the right hand side), as well as the heat convection and conduction:

$$\begin{aligned} & (\rho C_p)_{ef} \frac{\partial T}{\partial t} + (\rho^w C_p^w \mathbf{v}^{ws} + \rho^g C_p^g \mathbf{v}^{gs}) \cdot \operatorname{grad} T \\ & - \operatorname{div} (\chi_{ef} \operatorname{grad} T) = -\dot{m}_{vap} \Delta H_{vap} - \dot{m}_{prec} \Delta H_{prec} \end{aligned} \quad (3)$$

The latent heat transport is considered in the above equation by adding the product of water sink / source term due to evaporation / condensation, \dot{m}_{vap} , calculated based on eq. (3),

and the water phase change enthalpy, ΔH_{vap} . The precipitated salt mass source, $\dot{m}_{prec} = \dot{S}\phi\rho^p$, is obtained from the evolution equation (2) describing the salt precipitation / dissolution.

2.2. Salt phase change kinetics

It is assumed that there is no salt in the solid phase until the solution solubility limit ω_{sat} (i.e. the salt mass concentration of the saturated solution at a current temperature) is reached. After exceeding the maximum salt concentration the solution is supersaturated. An increase of solid salt mass is calculated on the basis of the supersaturation ratio, according to the following equation,

$$\frac{dS_p}{dt} = \begin{cases} S_w K(\omega - A'\omega_{sat})^p, & \omega \geq A'\omega_{sat} \wedge S_p < 1 \\ -S_w K|\omega - A'\omega_{sat}|^p, & \omega < A'\omega_{sat} \wedge 0 < S_p < 1 \end{cases} \quad (4)$$

3. Numerical simulation

The numerical example concerns the cooling and warming of 20 cm layer of cement mortar with the following physical properties: porosity $\phi = 0.12$, intrinsic permeability $k = 3.0 \cdot 10^{-21} \text{ m}^2$, specific heat $C_p = 840 \text{ J/(kg}\cdot\text{K)}$, thermal conductivity $\lambda = 0.82 \text{ W/m K}$, density $\rho = 2200 \text{ kg/m}^3$. The sample was fully saturated with sodium sulphate solution, whose initial concentration equals 0.28 [kg/kg]. The sodium sulphate saturation depends on the temperature:

$$\omega_{sat} = 0.0488\exp(0.0625\cdot\theta) \quad (5)$$

The above relation is valid for temperature $\theta \in [0, 32.4^\circ \text{C}]$. The crystal growth and dissolution were induced by the change of temperature of the ambient air:

$$\theta = \begin{cases} 30 - 10t, & t \in [0, 2] \\ 10, & t \in (2, 3) \\ -10 + 10t, & t \in [3, 5] \end{cases} \quad (6)$$

3.1. Numerical results

The boundary conditions are symmetrical therefore Figures 1,2,3 present the results only for the half of the analyzed element. Figure 1 presents the changes of the dissolved salt concentration profiles in the wall.

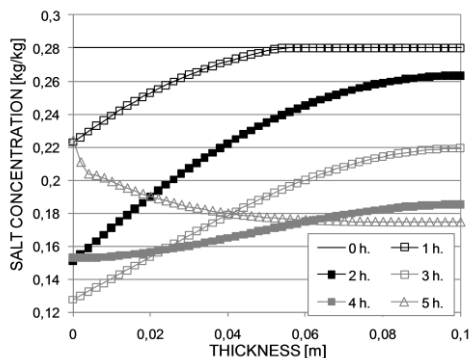


Figure 1. Profiles of the dissolved salt concentration.

For the first order rate law during the first period (cooling) the dissolved salt concentration rapidly decreases, whereas it sharply increases in the second period (warming) of the

analyzed process. During cooling the solution saturation rapidly decreases, according to eq.(5) and solution supersaturation ratio exceeds 1 – Figure 2. As a consequence the salt crystallization starts – Figure 3. During warming one can observe the increase of solution saturation and dissolution of crystals.

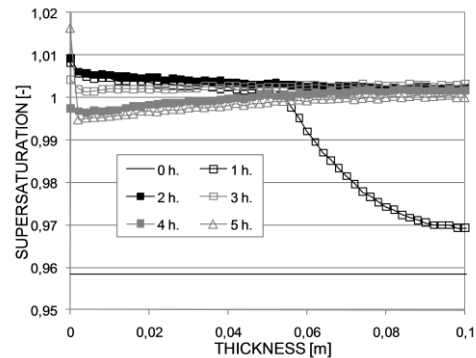


Figure 2. Profiles of the solution supersaturation ratio.

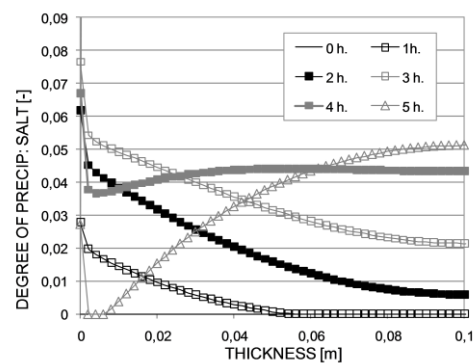


Figure 3. Profiles of the sat. degree with the precipitated salt.

4. Conclusions

The mathematical model describing moisture and salt transport in non-isothermal conditions was briefly presented in the paper. The process of salt phase change in the pore solution was modelled using the non-equilibrium approach, where the rate law describing mass change of the crystallized salt is known. During the cooling-warming experiment both the crystallization during the decrease of temperature and the dissolution of crystals during the increase of temperature can be noticed assuming the first and second order rate law.

References

- [1] Flatt, R.J., Steiger, M. and Scherer, G.W., A commented translation of the paper by C.W. Correns and W. Steinborn on crystallization pressure. *Environmental Geology*. 52, pp. 187-203, 2007.
- [2] Gawin, D. and Schrefler, B.A., Thermo-hydro-mechanical analysis of partially saturated porous materials. *Engineering Computations*. 13, pp. 113-143, 1996.
- [3] Koniorczyk, M. and Wojciechowski, M., Influence of salt on desorption isotherm and hygral state of cement mortar – Modelling using neural networks. *Constr. Build. Mater.* 23, pp. 2988-2996, 2009.
- [4] Bear, J. and Bachmat, Y., *Introduction to Modeling of Transport Phenomena in Porous Media*. Kluwer Academic Publishers, The Netherlands, 1991.