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Multiphysics model for spalling prediction of brick due to in-pore salt crystallization

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1. Introduction

There are several situations, when chemical degradation of porous building materials influences their durability to a great extent, like for example transport infrastructure exposed to deicing salts, harbor infrastructure and other constructions exposed to sea water, or historical structures after many years of exposure to natural climate and dissolution/crystallization of salts due to rain (which may be acid) and variable hygrothermal conditions.

Pores of building materials, such as concrete, natural stone, brick, are filled with gaseous (moist air) and/or liquid phases. Liquid phase consists of water with various chemicals dissolved in it, very often salts. Upon changes of external temperature and relative humidity the solution migrates through the material what may cause salt crystallization on the surface, called efflorescence, or inside the material, called subflorescence. Both types of salt crystallization are very dangerous. Efflorescence may lead to the chemical or physical degradation of the external layer, e.g. paintings or frescos, which belong often to the national heritage. Subflorescence causes the crystallization pressure, which may lead to internal cracking and finally to material delamination and spalling [1–3].

Recently a large amount of theoretical and experimental research was devoted to investigate the transport of dissolved salt in porous materials, salt phase change, and pressure which accompanies salt crystallization. A comprehensive theoretical framework for modeling coupled heat and mass transport in deformable porous materials was proposed in [4–6]. Following this general approach many authors developed mathematical models and numerical codes to analyze transport of salt and water in non-isothermal conditions [7–9]. Due to water evaporation or material cooling salts might crystallize. For the process analysis an accurate chemical model defining thermodynamic properties of a concentrated solution is needed. Such an approach was developed by Pitzer [10,11]. The Pitzer model parameters for sodium sulphate – water system were determined in [12,13]. The salt crystallization is accompanied by the crystallization pressure. There are generally two approaches for modeling crystallization pressure. The first one, started by Everett [14] and then further developed by Rodrigues et al. [1], is based on comparison of the chemical potential of crystals of

different size and curvature. The other one, derived from the Gibbs energy of a two phase system, defines the crystallization pressure as a function of salt activity. In the earlier works the activity was simplified by assuming to be equal to the solution concentration. An elegant thermodynamic derivation of crystallization pressure taking into account the crystal size was presented by Steiger [15,16].

Although some attempts were made in the past, there is still lack of a comprehensive mathematical model which would cover the material damage caused by salt crystallization, the proper definition of crystallization pressure in terms of ions activity and all sink/source terms appearing in the governing equations, due to salt phase change. In this paper we describe the extension of the formulation presented in [7] with an appropriate damage model and with the additional sink/source term appearing in the balance equations, related to the salt hydration process. Here two types of damage models are investigated: the static one and the delayed damage model. The comparison of the models and the limitations of the static one are presented. The advantages of a kinetic approach are underlined. In the paper we show the formulation of a delayed damage model, which is applied for the first time to the salt crystallization problem. The thermodynamic properties of the solution and the development of crystallization pressure in the confined pore system are discussed in detail. The coupled hygro-chemo-thermal model and some constitutive relations, which were presented in recent works, are briefly summarized for the convenience of the reader.

The effects of salt induced damage are very evident but they are also very sensitive to the chemo-physical conditions and therefore very difficult to measure. There are hardly any quantitative data in the literature dealing with salt crystallization. Therefore we will only validate the numerical procedure by performing the grid refinement test, and the sensitivity test on the kinetics of salt crystallization.

The outline of the paper is the following: after this introduction we present the brief derivation of crystallization pressure. The solution supersaturation ratio is defined based on the solution activity, which is calculated assuming the equilibrium between salt dissolved in water and solid salt. The relation between solution supersaturation ratio, temperature and salt concentration is given for sodium sulphate. Furthermore, we analyze the influence of pore size and shape on the salt solubility and crystallization pressure.

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List of symbols

a	ion activity [-]	r	process order (rate law) [-]
a_0	equilibrium activity of the crystal (possibly small crystal)	S	solution supersaturation ratio [-]
a_w	water activity [-]	S_π	saturation degree of the π - phase (volume occupied by the phase/volume of the pores), $\pi = W, A, P$ - liquid phase, gaseous phase, precipitated salt [-]
b	Biot's constant [-]	T	absolute temperature [K]
C_p	effective specific heat of porous medium [J/(kg K)]	t	time [s]
d	damage parameter [-]	\mathbf{t}'	effective stress tensor [Pa]
\mathbf{D}	stiffness tensor [Pa]	V_m	molar volume of salt [m ³ /mol]
D^{mol}	molecular diffusivity [m ² /s]	$\mathbf{v}^{\pi s}$	relative velocity π -phase ($\pi = W, A$ - liquid phase, gaseous phase) [m/s]
g	acceleration of gravity [m/s ²]	\mathbf{u}	the displacement vector [m]
ΔH_{vap}	enthalpy of vaporization per unit mass [J/kg]	x_s^{ws}	solid surface fraction in contact with the wetting film
ΔH_{prec}	enthalpy of crystallization per unit mass [J/kg]	Y	damage energy release rate
\mathbf{J}^{dysp}	dispersive flow of salt [kg/(m ² s)]	\mathbf{y}	primary variables nodal values vector,
\mathbf{J}_g^d	diffusive flux of dry air [kg/(m ² s)]		
\mathbf{J}_g^v	diffusive flux of water vapor [kg/(m s)]		
F	rate constant (rate law) [-]		
k	intrinsic permeability scalar [m ²]	<i>Greek symbols</i>	
$k^{\pi\pi}$	relative permeability of π - phase ($\pi = W, A$ - liquid phase, gaseous phase) [-]	β_s	cubic thermal expansion coefficient of the solid [1/K]
M_π	molar mass of π - compound [kg/kmol]	$\tilde{\gamma}_{cl}$	the mean surface free energy of the crystal-liquid interface [J/m ²]
$\frac{dm_{evap}}{dt}$	rate of mass due to evaporation [kg/(m ³ s)]	$\boldsymbol{\varepsilon}$	elastic strain tensor
$\frac{dm_{prec}}{dt}$	rate of mass due to crystallization [kg/(m ³ s)]	φ	strain energy density function [Pa]
$\frac{dm_{hydr}}{dt}$	rate of mass due to salt hydration [kg/(m ³ s)]	χ_{ef}	effective thermal conductivity [W/(m K)]
n	porosity (pore volume/total volume) [-]	μ^π	dynamic viscosity of π -phase ($\pi = W, A$ - liquid phase, gas) [Pa s]
p^π	pressure of ($\pi = W, A, P, V$ - liquid phase, gaseous phase, precipitated salt, water vapor) [Pa]	ρ^π	density of π -phase ($\pi = W, A, S, P$ - liquid phase, gaseous phase, solid skeleton, precipitated salt) [kg/m ³]
p^C	capillary pressure [Pa],	ρ^v	mass concentration of water vapor in gaseous phase [kg/m ³]
Δp	crystallization pressure [Pa]	ω	salt mass concentration in the solution [kg/kg]
R	universal gas constant (8314.41 J/(kmol K))		
RH	relative humidity [-]		

In the next section we include the description of the damage theory. Using thermodynamics of irreversible processes the constraint on damage parameters is defined. Two regularization methods are outlined: static one, based on the strain averaging and delayed damage theory. In the second approach we define the kinetic law for damage rate.

The model governing equations are derived in Section 3. Based on the Thermodynamically Constrained Averaging Theory (TCAT) we formulate the mass balance equation of the solid phase, air, water and salt, the energy balance equation and momentum balance equation. We formulate some most important constitutive relationships and outline the numerical methods, which are used to solve the problem.

In the last part, using the developed numerical model, we investigate the possible salt crystallization induced damage in brick. The discussion on the influence of the material microstructure on the salt crystallization is presented. After grid refinement test and sensitivity analysis we investigate the damage induced by salt crystallization in a wall due to the combination of water drying and cooling. We analyze two damage models and discuss the pros and cons of each of them. Due to very local character of salt crystallization it is very difficult to carry out the full experimental verification including strain analysis of the computational code. However, considering temperature variation due to salt crystallization in brick the presented model was verified against experimental data, see Koniorczyk and Konca [17].

2. Crystallization pressure

We assume that one salt only is dissolved in pore water. Nevertheless, the developed model is well suited to consider several salts

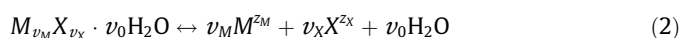
and various ions. The physical adsorption, due to van der Waals forces, of salt molecules by the solid skeleton is neglected, thus salt might crystallize and then salt crystals grow, only in the supersaturated solution. The thermodynamic properties of the concentrated solution are described by means of chemical potential. The model of crystallization pressure by Steiger [16] is followed. He considers the influence of the crystal size on the chemical potential, solubility and crystallization pressure. The solution supersaturation ratio is defined as follows:

$$S = \frac{a}{a_0} \quad (1)$$

where a is ion activity and a_0 is solubility product of small crystals of solid phase.

One of the most dangerous salts, causing the internal damage of building materials is sodium sulphate, Na₂SO₄, which will be considered in the present paper. Therefore, sodium sulphate - water system will be further analyzed. During the crystallization the deca-hydrate of sodium sulphate, called mirabilite, is formed Na₂SO₄ · 10H₂O - see Fig. 1.

Salt solution is an electrolyte containing cations (M) and anions (X). The dissociation reaction can be described as follows:



where z^+ indicates the charge of ions. The ion activity for hydrated salt is calculated according to

$$\ln a = v_M \ln(m_M) + v_X \ln(m_X) + v_M \ln(\gamma_M) + v_X \ln(\gamma_X) + v_0 \times \ln(a_w) \quad (3)$$

where v_i is the stoichiometric coefficient, m_i the molality, γ_i the ion activity coefficient for cation $i = M$ and anion $i = X$. The detailed

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