Journal of the Mechanics and Physics of Solids 63 (2014) 242–255

Contents lists available at ScienceDirect

Journal of the Mechanics and Physics of Solids

journal homepage: www.elsevier.com/locate/jmps

Deformation and damage due to drying-induced salt crystallization in porous limestone

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ARTICLE INFO

Article history:
Received 15 January 2013
Received in revised form
20 August 2013
Accepted 2 September 2013
Available online 16 September 2013

Keywords:
Salt crystallization
Fracture
Porous material
Finite elements
Nondestructive evaluation

ABSTRACT

This paper presents a computational model coupling heat, water and salt ion transport, salt crystallization, deformation and damage in porous materials. We focus on crystallization-induced damage. The theory of poromechanics is employed to relate stress, induced by crystallization processes or hygro-thermal origin, to the material's mechanical response. A non-local formulation is developed to describe the crystallization kinetics. The model performance is illustrated by simulating the damage caused by sodium chloride crystallization in a porous limestone. The results are compared with experimental observations based on neutron and X-ray imaging. The simulation results suggest that the crystallization kinetics in porous materials have to be accurately understood in order to be able to control salt damage. The results show that the effective stress caused by salt crystallization depends not only on the crystallization pressure but also on the amount of salt crystals, which is determined by the spreading of crystals in the porous material and the crystallization kinetics.

1. Introduction

Water and dissolved salt ions may penetrate into building materials due to diffusive and advective transport. Upon changes in the environmental conditions, salt can crystallize at the surface (efflorescence) or inside the material (subflorescence). Subflorescence is accompanied with the development of crystallization pressures, which may lead to spalling and cracking of the material, and thus to a reduction of the lifetime of a construction or monument. Until now, the mechanism of crystallization in confined conditions and the related damage processes, as well as the computational modeling, are still subject of scientific analysis. The availability of a model providing a full coupling between heat–water–salt ion transport, salt crystallization, deformations and damage would however be an important asset for engineers and conservators. It would allow them to assess and compare different maintenance, repair or conservation techniques or to assess the durability of a new building material under different climatic conditions, without having to perform long-term experiments.

Coupled numerical models for heat–water–salt transport and salt crystallization in building materials have been developed and described in the literature (Espinosa et al., 2007; Nicolai et al., 2007; Koniorczyk, 2012). Theories defining the

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http://dx.doi.org/10.1016/j.jmps.2013.09.005

crystallization pressure that is exerted when salt crystals grow in confined conditions are described as well (Scherer, 1999; Flatt, 2002; Steiger, 2005a, 2005b; Coussy, 2006). Moonen et al. (2010, 2011) developed a model that covers the effect of thermal and hygric changes on the damage behavior of porous media. There remains however a need for bringing together the available approaches within a single unifying framework. It is especially challenging to formulate the coupling between salt crystallization and the mechanical response of the building material and to accurately model the crystallization kinetics in a physically and numerically sound way.

In the next section, we present a fully coupled model for heat, water and salt ion transport, salt crystallization, material deformation and damage in porous media. We briefly recall the modeling of heat and moisture transport (Derluyn, 2012). The modeling of the salt crystallization process, the coupling with the mechanical behavior and the damage criterion are discussed in more detail. In Section 3, we summarize experimental observations of damage caused by sodium chloride crystallization, induced by drying of an initially wet limestone (Derluyn, 2012). The material and salt properties, needed as input for the model, are also given. Section 4 comprises the simulation of the performed experiment. Comparison with the experimental data suggests that the crystallization kinetics play an important role in the accurate prediction of salt damage.

2. A coupled model for transport, crystallization, deformation and damage

2.1. Conservation of mass

We consider the porous medium consisting of a superposition of four phases: (1) the solid material matrix, (2) the gas phase, (3) the liquid phase and (4) the crystal phase. In these phases several components can be present. For the gas phase we consider dry air and water vapor, for the liquid phase water and dissolved salt ions. Exchange of water can occur between the liquid and the gas phase due to evaporation or condensation, or between the liquid and the crystal phase when hydrated salt crystals form or dissolve. Exchange of salt ions occurs between the liquid and the crystal phase when crystals precipitate or dissolve. We assume that the dissolved salt does not separate macroscopically in the absence of an electric field. Thus the cations and anions are always transported jointly.

We further assume that the solid phase does not exchange mass with other phases. We consider the gas pressure, p_g, to be constant and equal to the atmospheric pressure. In addition, we consider changes in the water vapor mass to be negligible with respect to changes in the liquid water mass and we assume that salt crystals do not move in the pore space.

Under these assumptions, the mass balance is expressed by

$$\Phi\frac{\partial(S_l\rho_l+S_{cr}\rho_{cr})}{\partial t}=\nabla\cdot(\mathbf{K}_l\nabla p_c+\boldsymbol{\delta}_v\nabla p_v) \tag{1}$$

with Φ the total accessible porosity, S_l and S_{cr} the liquid and the crystal saturation degree, respectively, and ρ_l and ρ_{cr} the density of the liquid phase and of the salt crystal. $\mathbf{K}_l$ is the liquid permeability as function of capillary pressure p_c. The capillary pressure expresses the pressure difference across the liquid–gas interface and is defined as

$$p_c=p_l-p_g \tag{2}$$

with p_l the liquid pressure and p_g the (constant) gas pressure. $\boldsymbol{\delta}_v$ is the vapor permeability in function of vapor pressure p_v. The vapor pressure can be expressed in terms of the capillary pressure p_c, the absolute temperature T and the water activity a_w by the modified Kelvin relation

$$p_v=a_w p_{v,sat}\exp\left(\frac{p_c}{\rho_w R_v T}\right) \tag{3}$$

with $p_{v,sat}$ the saturated vapor pressure, ρ_w the water density and R_v the gas constant for water vapor. The water activity depends on the temperature and the salt concentration and accounts for the change of the vapor pressure in equilibrium with a salt solution, compared to the vapor pressure in equilibrium with pure water. For pure water, the water activity equals 1. The higher the salt concentration gets, the lower the water activity will be, leading to lower vapor pressures.

Under the assumption that the dissolved salt ions are transported together, the mass balance for the salt dissolved in the liquid phase reads

$$\Phi\frac{\partial(S_l\rho_l C)}{\partial t}+\Phi\frac{\partial S_{cr}/\overline{V}_{cr}}{\partial t}=\nabla\cdot(\rho_l\mathbf{D}_i^l\nabla C)+\nabla\cdot(C\mathbf{K}_l\nabla p_c) \tag{4}$$

with C the salt concentration in mole/kg liquid solution and $\overline{V}_{cr}$ the molar volume of the salt crystal. $\mathbf{D}_i^l$ is the salt diffusion coefficient in the liquid phase.

2.2. Conservation of energy

The global energy balance for the porous medium reads

$$\frac{\partial(((1-\Phi)c_{p,s}\rho_s+\Phi c_{p,l}S_l\rho_l+\Phi c_{p,cr}S_{cr}\rho_{cr})(T-T_0))}{\partial t}+\frac{\partial\Phi L_{cr}S_{cr}\rho_{cr}}{\partial t}+\nabla\cdot\mathbf{q}_e=0 \tag{5}$$