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Ice-induced damage of cement based composites – experimental and numerical study

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Abstract

The paper considers water solidification in porous materials. Mathematical model describing heat and water transport in deformable porous materials considering the kinetics of water phase change was proposed. The crystallization pressure was determine using the volume averaged Everett's equation. The ice-induced destruction of concrete was modeled by means of the delayed damage approach. The numerical code was developed using finite element, finite difference and Newton-Raphson methods.

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Keywords: frost damage; porous building materials; durability; numerical simulations.

1. Introduction

Cyclic freezing of water in porous building materials is one of the most destructive phenomena strongly influencing the building structures durability. The main reason of frost damage is the increase of molar volume of ice when compared to the one of water. Ice growth induces additional pressure acting on the material skeleton but it also increases liquid water pressure, what is even more severe for the material durability.

A mathematical model of coupled heat and moisture transfer and frost deterioration in a fully water saturated porous material, exposed to freezing/thawing cycles, is formulated by means of mechanics of multiphase porous media. The mathematical model of coupled heat and water transfer in deformable porous media, considers water freezing/melting and crystallization pressure exerted by the processes, causing material deterioration. The kinetics of phase transformation was modelled by means of non-equilibrium approach, which was previously applied for salt crystallization [1, 2] and leaching of calcium in cementitious materials [3]. The frost deterioration was modelled by

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means of isotropic nonlocal damage theory of Mazars [4-7]. Here a rate formulation of the damage model was used, see e.g. [8, 9]. The model equations were solved numerically by means of the research computer code.

Nomenclature

b	Biot number
d	damage coefficient
T	temperature
p^C, p^L	crystallization-, liquid- pressure
K_S, K_L, K_C	skeleton-, liquid-, ice- bulk modulus
ϕ	porosity
ρ^C, ρ^L	ice-, liquid- density
η_C, η_L	relative content of ice, liquid in the pore system
$\mathbf{v}^{LS}$	velocity of liquid relative to the skeleton
$\mathbf{v}^S$	velocity of the skeleton

2. Mathematical model

Porous material is modeled as a multiphase deformable medium. It is assumed that the voids are filled with water or when temperature is below the water freezing point, partly with ice and partly with yet unfrozen water. The mathematical model consists of three balance equation: mass balance of water molecules, energy balance and linear momentum balance. Therefore, three following state variables are chosen: liquid pressure, p^L, temperature, T and displacement vector, $\mathbf{u}$. The mathematical model must be complemented with ice crystals evolution law, which is defined by means of degree of pore saturation with ice, η_C.

Applying the equation defining the material derivative of porosity, the state equation of water and ice and introducing the definition of the pressure exerted by the phases occupying pores on the solid skeleton as: $p^S = \eta_L p^L + \eta_C p^C = = p^L + \eta_C \left(p^C - p^L \right)$, one can derived the final form of matter mass balance equation as follows:

$$\begin{aligned}
&\left\{ \phi(1-\eta_C)\frac{\rho^L}{K_L} + \phi\eta_C\frac{\rho^C}{K_C} + \left[\eta_C\rho^C + (1-\eta_C)\rho^C\right]\frac{(b-\phi)}{K_S} \right\}\frac{D^S p^L}{Dt} + \\
&+\left\{ \phi\eta_C\frac{\rho^C}{K_C} + \eta_C\left[\eta_C\rho^C + (1-\eta_C)\rho^C\right]\frac{(b-\phi)}{K_S} \right\}\frac{D^S}{Dt}\left(p^C - p^L\right) + \\
&+\left\{ \phi\eta_C\beta_C\rho^C + \phi(1-\eta_C)\beta_L\rho^L - \beta_S\left[\eta_C\rho^C + (1-\eta_C)\rho^C\right](b-\phi) \right\}\frac{D^S T}{Dt} + \\
&\left\{ \phi\left(\rho^C - \rho^L\right) + \left[\eta_C\rho^C + (1-\eta_C)\rho^C\right]\left(p^C - p^L\right)\frac{(b-\phi)}{K_S} \right\}\frac{D^S\eta_C}{Dt} + \nabla\cdot\left(\phi\eta_L\rho^L\mathbf{v}^{LS}\right) + \\
&+\left\{ \phi(1-\eta_C)\rho^L + \phi\eta_C\rho^C + \left[\eta_C\rho^C + (1-\eta_C)\rho^C\right](b-\phi) \right\}\nabla\cdot\mathbf{v}^S = 0
\end{aligned} \tag{1}$$

The energy conservation equation written for the multiphase domain, considering the kinetics of water/ice phase change and the energy sink/source related to that transformation, and neglecting the convective term, reads:

$$(\rho C)_{ef}\frac{D^S T}{Dt} = \nabla\cdot\left(\lambda_{ef}\nabla T\right) + \rho_C\Delta H\frac{D^S\eta_C}{Dt} \tag{2}$$

where $(\rho C_p)_{ef}$ and λ_{ef} are the effective values of thermal capacity and thermal conductivity of the multiphase material and ΔH is the volumetric latent heat of water solidification, equal to 333 J/g. The momentum balance equation reads:

$$\nabla \cdot \left(\mathbf{t}^{\text{total}} \right) + \mathbf{g} \left[(1-\phi)\rho^S + \phi \eta_L \rho^L + \phi \eta_C \rho^C \right] = 0 \tag{3}$$

Considering the mechanical behavior of porous material it is necessary to take into account both the effects of an external load and the pressure exerted on the skeleton by phases occupying its voids (water and ice pressure). Hence, the total stress tensor $\mathbf{t}^{\text{total}}$ acting in a point of the porous medium may be split into the effective stress $\mathbf{t}_e^S$, and a part, which accounts for the pressure exerted by the pore fluids, p^S:

$$\mathbf{t}^{\text{total}} = \mathbf{t}_e^S - b\, p^S \mathbf{I} \tag{4}$$

where the effective stress is given by the formula:

$$\mathbf{t}_e^S = (1-d)\,\mathbf{D}\left(\boldsymbol{\varepsilon}_{tot} - \boldsymbol{\varepsilon}_T \right) \tag{5}$$

To describe the rapture of material, we chose the delayed damage model proposed by [10, 11] which was successfully applied for dynamic problems [8, 9], and which reads:

$$\dot{d} = \frac{1}{\tau_c} \left[1 - \exp\left(-a \left\langle g(\kappa) - d \right\rangle \right) \right] \tag{6}$$

where the damage law might be given by the relations [6]:

$$g(\kappa) = 1 - \frac{\varepsilon_0}{\kappa} \exp\left(-\frac{\kappa - \varepsilon_0}{\varepsilon_f} \right) \quad \textit{for } \kappa \geq \varepsilon_0 \tag{7}$$

where ε_0 is the elastic strain limit, ε_f is the parameter controlling the post-peak slope of stress-strain curve,

$$\kappa(t) = \max_{\tau \leq t} \tilde{\varepsilon}(\tau) \tag{8}$$

The ice content depends on the temperature but also on the radius of the pores where the crystals currently grow. Ice does not appear suddenly in the pore space but it is a process consisting of two parts. The rate of ice growing might calculated by the equation proposed by Bronfenbrener and Korin [12], which was adopted for the proposed formulation:

$$\dot{\eta}_C = \frac{\eta_C^{\,EQ} - \eta_C}{\tau} \tag{9}$$

where η_C^{EQ} is the ice content calculated for the equilibrium condition at the temperature T.

The average crystallization pressure exerted by ice on the material skeleton, $\left\langle \eta_C\, p^C \right\rangle$, considering its cumulative pore size distribution curve, $V(r)$, was calculated by means of the theory developed by Monteiro and Coussy [13],

$$\left\langle \eta_C p^C \right\rangle = \frac{\gamma_{CL}}{\phi} \int_{\infty}^{R} \left(\frac{2}{R} - \frac{2}{r} \right) \frac{dV(r)}{dr} dr \,, \tag{10}$$

where γ_{CL} means the surface tension of water – ice interface. The effect of damage on the crystallization pressure (10) was considered by means of the pore size distribution curves measured with MIP for frost-deteriorated material.

3. Numerical solution

The mathematical model, eq. (1-3), consists of three coupled PDEs, which were solved using appropriate numerical method. Galerkin approximation was applied to the weak form of governing PDEs. Space integration is carried out using the Finite Element Method [14]. The isoparametric formulation was aliped so, the same interpolation function were used to determine the elements geometry as were used to calculate the primary variable field. The weak form of the model equations after applying Stokes Theorem, integration by parts and assuming that the skeleton velocity is negligible small, reads:

$$\begin{bmatrix} C_{LL} & C_{LT} & C_{L\mathbf{u}} \\ C_{TL} & C_{TT} & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{Bmatrix} \dot{\bar{p}}_L \\ \dot{\bar{T}} \\ \dot{\bar{\mathbf{u}}} \end{Bmatrix} + \begin{bmatrix} K_{LL} & 0 & 0 \\ 0 & K_{TT} & 0 \\ K_{\mathbf{u}L} & K_{\mathbf{u}T} & K_{\mathbf{uu}} \end{bmatrix} \begin{Bmatrix} \bar{p}_L \\ \bar{T} \\ \bar{\mathbf{u}} \end{Bmatrix} = \begin{Bmatrix} f_L \\ f_T \\ f_{\mathbf{u}} \end{Bmatrix} \tag{11}$$

Assuming the vector of unknowns $\mathbf{x} = [\bar{\mathbf{p}}_L, \bar{\mathbf{T}}, \bar{\mathbf{u}}]$, the set of governing equations might be written in the compact form:

$$\mathbf{C}(\mathbf{x}) \frac{\partial \mathbf{x}}{\partial t} + \mathbf{K}(\mathbf{x})\mathbf{x} = \mathbf{f}(\mathbf{x}) \tag{12}$$

Most of material properties depends on the current state of the system, therefore (12) represents the nonlinear set of ordinary differential equations. The time integration was done by means of fully implicit Finite Difference Method (backward Euler algorithm):

$$\mathbf{\Psi}^i(\mathbf{x}_{n+1}) = \mathbf{C}_{ij}(\mathbf{x}_{n+1}) \frac{\mathbf{x}_{n+1} - \mathbf{x}_n}{\Delta t} + \mathbf{K}_{ij}(\mathbf{x}_{n+1})\mathbf{x}_{n+1} - \mathbf{f}_i(\mathbf{x}_{n+1}) = 0 \tag{13}$$

where $i,j = L,T,\boldsymbol{u}$, n is time step number and Δt is time step length. The set of differential, non-linear equations (13) is solved by means of a monolithic Newton-Raphson type iterative procedure [14]:

$$\mathbf{\Psi}^i(\mathbf{x}_{n+1}^l) = -\left.\frac{\partial \mathbf{\Psi}^i}{\partial \mathbf{x}}\right|_{\mathbf{x}_{n+1}^l} \Delta \mathbf{x}_{n+1}^l; \qquad \mathbf{x}_{n+1}^{l+1} = \mathbf{x}_{n+1}^l + \Delta \mathbf{x}_{n+1}^l \tag{14}$$

where l is iteration index.

4. Modeling frost-induced damage of a concrete wall

The problem concerns frost damage of a concrete wall exposed to the two-sided cyclic variation of temperature. The 20-cm wall, initially fully saturated with water, was considered. Due to the symmetry of boundary condition, only half of the wall was analyzed, assuming zero fluxes on the axis of symmetry. The analyzed domain was divided into 100 tetragonal finite elements of equal size. The following material parameters were assumed in simulation: porosity $\phi = 6\%$, thermal conductivity $\lambda = 1.5$ W/(m·K), intrinsic permeability $k = 3\cdot10^{-21}$ m^2, Young modulus $E = 25$ GPa, compressive strength f_{ct} = 3.0 MPa. The convective (Robin) boundary conditions were assumed for heat transport with the heat transfer coefficient h = 8 W/(m^{2}K). The ambient temperature variation is described by the formula:

$$T=\begin{cases}293.15-8t\left[K\right],\ t\in\left[0h,5h\right)\\ 253.15\left[K\right],\ t\in\left[5h,10h\right)\\ 253.15+8\left(t-10\right)\left[K\right],\ t\in\left[10h,15h\right)\\ 293.15\left[K\right],\ t\in\left[15h,20h\right]\end{cases} \tag{14}$$

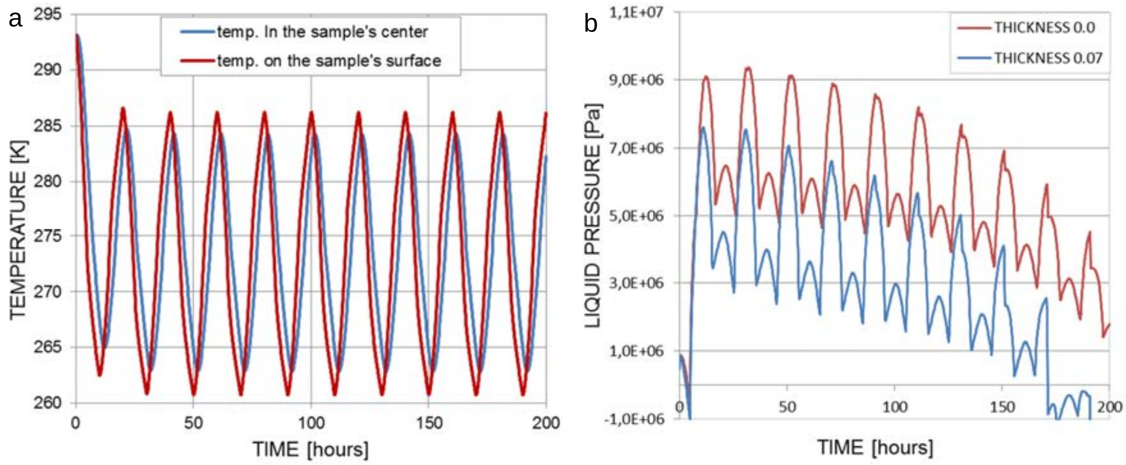

Fig. 1. The simulation results concerning evolution of: (a) temperature; (b) liquid water pressure; in two points of a concrete wall.

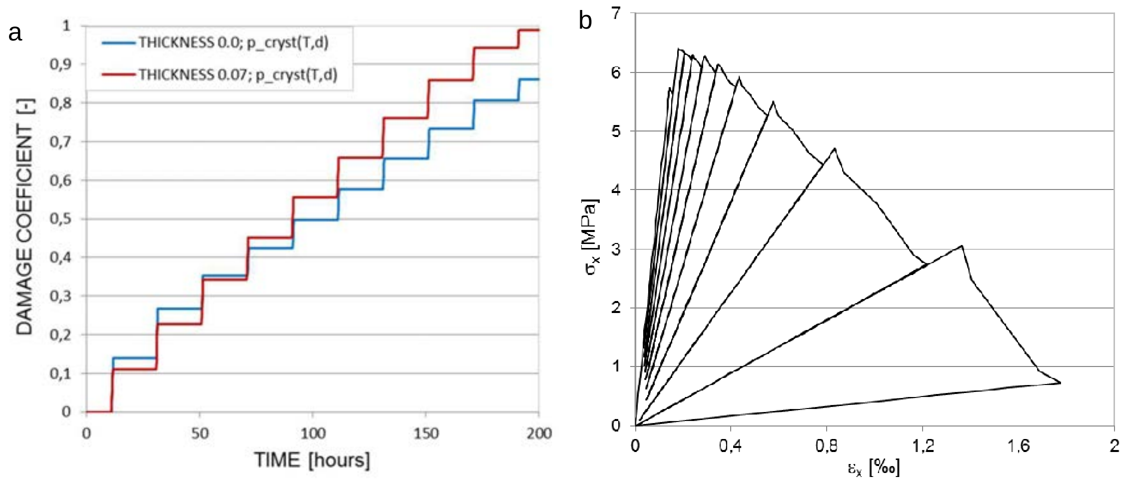

Fig. 2. The simulation results concerning evolution of: (a) temperature in two points of a concrete wall; (b) strain – stress performance.

The total simulation time was equal to 200 h thus it comprised the 10 temperature cycles. The computed time evolutions of temperature and liquid water in two points of the wall, on its surface and 7 cm from it (marked as "in center"), are presented in Figure 1. As can be observed in Fig. 1a, after the first cycle the temperature changes were periodically repeated with the same amplitude. The temperatures on the wall surface and in the whole wall were very similar, and no distinct effects of water phase transitions were observed due to their spreading over a range of temperatures. On the contrary to temperature, the amplitude of water pressure oscillations was gradually decreasing due to frost damage increasing after every freezing/thawing cycle, having slightly higher value inside the wall, see Fig. 2a. During every cycle, the water pressure was initially increasing due to water freezing and related increase of water molar volume. Then it was decreasing due to ice melting and related decrease of its volume, up to the moment when the phase change was completed and further changes of water pressure were caused by different thermal dilatation of water and skeleton. Since the skeleton strength properties were gradually degrading (Fig. 2b), due to progressing frost induced material damage, to a more extent inside the wall (Fig. 2a), the water pressure amplitude was lower inside the wall. The frost induced material damage is caused mainly by high value of crystallization pressure exerted by ice on the material skeleton. Since damage (material cracking) changes a material pore size distribution, causing an increase of larger pores volume, the crystallization pressure accordingly increases, see eq. (10) causing further progress of frost damage. The process is more pronounced inside the wall. In practice, surface layers of a building envelope are more exposed to very high moisture content (even to fully saturated conditions), associated by low temperatures (below pore water freezing temperature), hence surface layer is more jeopardized by frost damage, causing spalling of thin material flakes.

5. Conclusions and final remarks

A mathematical model allowing for analysis of frost damage of porous building materials, the pores of which are fully saturated with water, was presented. The model equations were numerically solved and the research code was developed. The presented simulation results allow for better understanding of physical mechanisms of frost damage of porous building materials. Further developments of the model and its experimental validation are in progress.

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