Modeling freezing of partially saturated cementitious materials with considering process kinetics

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ABSTRACT

In this work we present a new numerical model of hygro-thermal processes in a porous material, partially or fully saturated with liquid water, exposed to temperatures below the freezing point of pore water. Water freezing in a capillary-porous material is a very complex physicochemical process, rather difficult to model numerically. In modelling the assumption that there exists thermodynamic equilibrium between the solid (ice) and liquid phases of water is usually applied. Thanks to this assumption, in the simulations one can use the equilibrium curve, which describes liquid water content in the material pores (or the saturation degree with liquid water $S_w^{eq}\left(T\right)$) being in equilibrium with the solid water (ice) at a given temperature T during very slow freezing. Here the water freezing / melting in the material pores is modeled as a non-equilibrium process (but close to thermodynamic equilibrium), which kinetics is governed by the linear evolution law, obtained from the second law of Thermodynamics. During freezing of water in a partially saturated porous material (i.e. filled partly with gas phase), liquid water occupies the whole volume of pores with the smallest radii, while ice is formed at the interface between liquid and solid water (gradually progressing into finer pores) and on the ice / gas interface. The liquid water can flow through a thin film of physically adsorbed water between the skeleton and ice crystal [1, 2], hence water pressure does not increase during freezing in a partially saturated material.

As far as the effective stress principle is concerned, at temperatures when only liquid water and moist air are present in the pores (i.e. no ice is present), a usual relation between the water pressure and gas pressure, considering also disjoining pressure. During freezing of water at thermodynamic equilibrium, the pressure difference on the interface between ice and liquid water in the pores can calculated by means of the Gibbs-Thomson law [1]. The crystallization pressure, exerted on material skeleton by a crystal of ice situated in a pore can be derived by the relationships proposed by Scherer [2]. With these measures of pressure it is possible to evaluate the effective stress on the solid skeleton of the porous medium due to the simultaneous presence of gas, water and ice.

Some relevant numerical cases will be presented to show the effectiveness of the formulated model.

REFERENCES

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[2] Z. Sun, G.W. Scherer, "Effect of air voids on salt scaling and internal freezing", *Cement and Concrete Research*, Vol. **40**, pp. 260–270, (2010).