Modeling of ice formation in porous solids with regard to the description of frost damage

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Abstract

The freezing and thawing of liquid in porous media in connection with the question concerning the frost durability of solid materials is an important subject for discussion in civil engineering. Each construction or body which is in contact with liquid and frozen water is criticized by its resistance to the environment. The durability concerning frost attacks of a building material is affected by its porosity and the pore size distribution. The ice formation is a phenomenon of coupled heat and mass transport in freezing porous media, and is primarily caused by the expansion of ice in connection with hydraulic pressure. The volume increases due to the freezing front inside the porous solid. Taking into account the aforementioned effects in porous materials, a simplified macroscopic model within the framework of the Theory of Porous Media (TPM) for the numerical simulation of initial and boundary value problems of freezing and thawing processes of super saturated porous solids will be presented. The phase change between the ice and the liquid phase is modeled by different real densities of the phases.

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1. Introduction

Transport phenomena with and without phase transition in porous media are encountered, e.g., in civil engineering. Examples include the drying of porous solids, the freezing of soils, the geothermal application, etc. One of the main issues in material science is the frost resistance of solid materials. Each construction is criticized by its resistance to the environment. Therefore, frost attack is divided into two main types: (i) internal frost attack caused by the freezing of a liquid phase inside the material; (ii) surface scaling, normally caused by the freezing of weak salt solutions at the surface of the solid matrix. The two types of attack depend on the same basic mechanism,
namely, that too much liquid is present in the pores. It has been shown that after a high number of freeze-thaw cycles frost damage is not a fatigue mechanism, see [13].

In the present paper a coupled heat and moisture flux in a porous solid matrix will be simulated by using the Theory of Porous Media (TPM). Therefore, a representative unit cell of the solid matrix will be considered. The “representative unit cell” is a material volume that is big enough to represent the material in bulk, but not much bigger than that, i.e., it shall be big enough to contain the same porosity and the same pore size distribution as the material in bulk. The exchange between the ice and liquid phase is modeled by the different real densities of the phases. During the phase change a mass transport from liquid to ice and vice versa takes place.

2. Basics

The basics of the TPM are the concept of volume fractions in connection with the saturation condition, the kinematics, the balance equations and the entropy inequality in view of the derivation of restrictions for constitutive relations. These basics will be discussed in the following.

2.1. The concept of volume fraction and saturation condition

The concept of volume fractions in addition to the mixture theory has shown itself to be an efficient tool for investigating saturated as well as empty porous solids. With the assumption that the pores are statistically distributed over the porous solid, this concept effects the distribution of the mass of the constituents over the control space of solid. Thus, with the concept of volume fractions the single constituents are “smeared” over the control space of the solid phase and occupy the whole volume of the control space simultaneously. The “smeared” substitute continua (partial bodies) show the same properties as a mixture body, so that the mixture theory is the most adequate basis for a thermodynamic treatment of porous media at the macroscale.

In contrast to mixtures, with respect to the description of porous media, it is of essential importance that the partial bodies of a porous medium be “identifiable” at any time during a thermodynamic process. The identification will be done with the help of the concept of volume fractions.

As mentioned, it will be assumed that each constituent (phase) \( \varphi^a \) would occupy any point \( \mathbf{x} \) at any time \( t \). Furthermore, a real density \( \rho^a^{\text{R}}(\mathbf{x}, t) \) as well as a volume fraction \( n^a(\mathbf{x}, t) \) will be assigned to each phase. The real density of a constituent is the mass of \( \varphi^a \) per unit volume \( \text{d}v^a \), while the volume fraction \( n^a = \text{d}v^a / \text{d}v \) of a phase \( \varphi^a \) represents the proportion of the total volume occupied by the constituent. The partial density \( \rho^a \) of the phase \( \varphi^a \) is determined by

\[
\rho^a = n^a \rho^a^{\text{R}}. \tag{1}
\]

The real density is a quantity which transfers one important material behavior from the microscale to the macroscale, i.e., whether the real material of a constituent is incompressible or compressible, or rather, whether the real density of the constituent is constant or not.

Since the solid particles and all remaining \( \kappa - 1 \) constituents are assumed to occupy all the volume available, the porous solid is said to be saturated and

\[
\sum_{a=1}^{\kappa} n^a = 1. \tag{2}
\]

Eq. (2) is the so-called saturation condition, which plays an important role in the TPM because this condition restricts the motion of the individual phases.

2.2. Kinematics

Within the framework of the general porous media theory, a saturated porous medium will be treated as an immiscible mixture of all constituents \( \varphi^a \) with particles \( \mathbf{X}_a \), where at any time \( t \) each spatial point of the current placement of the solid phase is simultaneously occupied by particles \( \mathbf{X}_a \) of all constituents. These particles proceed from different reference positions \( \mathbf{X}_a \) at time \( t = t_0 \). Thus,
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