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A micromechanics model for partial freezing in porous media

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ABSTRACT

Based on the local physical characterization of partial freezing in porous media, the role of the unfrozen water film, located between the in-pore ice crystal and pore wall, is paid special attention to in this study. The disjoining pressure within unfrozen water film, the membrane stress induced by surface tension effect, the thermal stress and the initial stress are fully accounted for in the proposed micromechanics model. The micromechanics model improves the physical understanding of the macroscopic mechanical behaviors of the partially frozen porous media. The micromechanics model is applied to simulate the free swelling of a undrained cement paste (denoted by CP) and an air-entrained mortar (denoted by AM). The model results are comparable with the experimental results on cement paste. The reasons for the discrepancies between the model results and experimental results on cement paste may lie in the overestimation of the ice content, which here is estimated by the pore size distribution by mercury intrusion porosimetry (MIP) and Gibbs–Thomson equation. However, the model results agree well with the experimental results of the air-entrained mortar, the ice content of which is determined by the differential scanning calorimeter (DSC). The disjoining pressure within partially frozen porous media will become more and more significant with decreasing temperature.

1. Introduction

Internal frost damage and surface scaling damage are considered to be the two main deteriorating phenomena of concrete structure in cold region, which is more and more concerned by the civil engineering community (Sun and Scherer, 2010a). After the pioneering work of Powers and Helmuth (1953), numerous models were developed to investigate the mechanism of the deterioration as well as to simulate the mechanical behaviors of the frozen porous media (Scherer, 1999; Zuber and Marchand, 2004; Coussy, 2005; Coussy, 2006; Coussy and Monteiro, 2008; Wardeh and Perrin, 2008; Sun and Scherer, 2010a; Zeng et al., 2011b; Fen-Chong et al., 2013a,b). In these models, poromechanics models developed by Coussy and coworkers (Coussy, 2005; Coussy, 2006; Coussy and Monteiro, 2008; Fen-Chong et al., 2013a,b) have been proved to be robust and comprehensive for studying the behaviors of partially frozen porous media. Based on the thermodynamic equilibrium of in-pore ice crystal, "crystallization pressure" is introduced in the poromechanics model for partially frozen porous media by Scherer et al. (Scherer, 1999; Sun and Scherer, 2010a). In the previous poromechanics models, the local physics information (e.g. disjoining pressure in unfrozen water film) along with heterogeneous microstructure of frozen porous medium are not fully taken into account at local scale in these models.

The existence of the unfrozen water film, located between ice crystal and pore wall, has been verified by extensive works (Faraday, 1859; Fagerlund, 1973; Derjaguin et al., 1987; Churaev et al., 1994; Scherer and Valenza, 2005). Therefore, in crystallized pores, the unfrozen water film instead of ice crystal directly exerts pressure on the pore wall (see Fig. 1). Moreover, an additional pressure denoted as "disjoining pressure" emerges in this unfrozen water film, which is believed to play a crucial role in mechanical behaviors of partially frozen porous media (Derjaguin and Obuchov, 1936; Derjaguin and Churaev, 1978; Derjaguin et al., 1987; Churaev et al., 1994). This local physical information is always not accounted for in the poromechanics models, as explained in Coussy (2006).

As an alternative approach for poromechanical approach, micromechanics approach has already been used to model the mechanical behavior of unsaturated porous medium (Chateau et al., 2002; Cariou, 2010). The micromechanics methodology is capable of accounting for the heterogeneous microstructure as well as local physical behavior. By means of the homogenization and appropriate estimate scheme (e.g. Mori–Tanaka scheme in this

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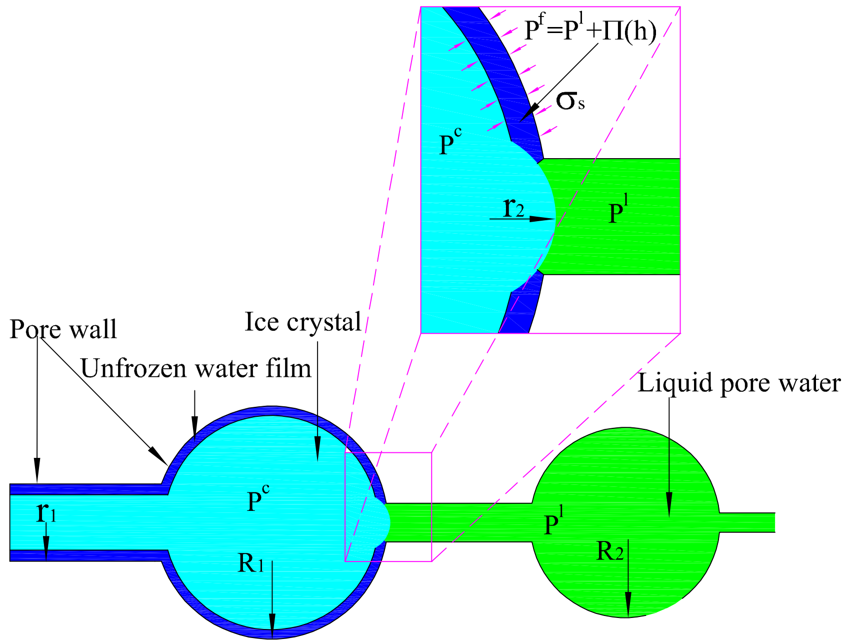

Fig. 1. Schematic illustration of partial freezing within porous media.

study), the micromechanics model is able to characterize the macroscopic behaviors of the partially frozen porous media. Moreover, it also allows us to discuss the impact of local physical quantity (such as the disjoining pressure in this study) on the macroscopic behaviors during freezing in porous media.

The aim of this study is devoted to developing a comprehensive model for partial freezing in porous media by means of the micromechanics methodology. The effect of unfrozen water film and the disjoining pressure is emphasized in the model. The paper is organized as follows: Section 2 recalls the physical characterization of the partial freezing in porous media; based on this physical characterization, the two state equations of the micromechanics model are presented in Section 3. In Section 4, the two state equations are used to discuss and interpret the macroscopic behavior of the partially frozen porous medium in isotropic case; in Section 5, the micromechanics model is also employed to model the free swelling of the partial frozen cement paste and air-entrained mortar. this context, the curlicue letters represent fourth order tensor (e.g. $\mathbb{C}, \mathbb{A}$), the boldfaced letters denote second order tensor (e.g. $\boldsymbol{\sigma}, \boldsymbol{E}$) while underlined letters (e.g. $\underline{\xi}, \underline{n}$) denote vectors. The subscripts and/or superscripts of s, c, l, f, cf and p represent solid matrix, ice crystal, liquid pore water, unfrozen water film, unfrozen water film + ice crystal composite and pore space, respectively.

2. Local physical characterization

As shown in Fig. 1, the partial freezing in porous media can be treated as unsaturated case in which the ice crystal is non-wetting phase and the liquid pore water is wetting phase. Therefore, during freezing process, the physics within interfaces (e.g. ice crystal-liquid pore water interface $\mathcal{I}^{cl}$) and the unfrozen water film f (as shown in the subset of Fig. 1) should be paid special attention to at local scale.

2.1. The interfaces in partially frozen porous media

As can be seen in Fig. 1, during freezing process, there exist four interfaces: pore wall/liquid pore water interface ($\mathcal{I}^{sl}$), pore wall/unfrozen water film interface ($\mathcal{I}^{sf}$), ice crystal/liquid pore water interface ($\mathcal{I}^{cl}$) and ice crystal/unfrozen water film interface ($\mathcal{I}^{cf}$). The surface tension $\gamma_{\alpha\beta}$ along a interface $\mathcal{I}^{\alpha\beta}$ induces a stress vector discontinuity ($[\boldsymbol{\sigma}].\underline{n}$) between α and β phases, ($\alpha, \beta \in l, s, f, c$); where $\underline{n}$ is the unit vector normal to the interface $\mathcal{I}^{\alpha\beta}$ between the α phase and β phase; $[\boldsymbol{\sigma}]$ is the stress difference between α phase and β phase. If we assume $\underline{n}$ orientates towards α phase, then $[\boldsymbol{\sigma}] = \boldsymbol{\sigma}^\alpha - \boldsymbol{\sigma}^\beta, \boldsymbol{\sigma}^\alpha$ and $\boldsymbol{\sigma}^\beta$ are the local stress tensors within α phase and β phase, respectively. It should be noted that, herein, $\boldsymbol{\sigma}$ is concise expression of $\boldsymbol{\sigma}(\underline{z}), \underline{z}$ is local position vector. With the introduction of the curvature tensor of interface, defined by $\boldsymbol{b} = -\text{grad}\underline{n}$, the stress vector discontinuity can be derived from the momentum balance equation (Dormieux et al., 2006):

$$[\boldsymbol{\sigma}].\underline{n} + \gamma_{\alpha\beta}(\mathbf{1}_T : \boldsymbol{b})\underline{n} = 0 \tag{1}$$

where $\mathbf{1}_T$ ($\mathbf{1}_T = \mathbf{1} - \underline{n} \otimes \underline{n}$) is the second order identity tensor of the plane tangent to the interface $\mathcal{I}^{\alpha\beta}, \mathbf{1}$ is the second order identity tensor.

For the ice crystal-liquid pore water interface ($\mathcal{I}^{cl}$), $\boldsymbol{\sigma}^c = -P^c\mathbf{1}, \boldsymbol{\sigma}^l = -P^l\mathbf{1}, [\boldsymbol{\sigma}] = \boldsymbol{\sigma}^c - \boldsymbol{\sigma}^l$, Eq. (1) can thus be rearranged as the classic Young–Laplace equation:

$$P^c - P^l = \kappa_{cl}\gamma_{cl} \tag{2}$$

where P^c and P^l are the pressures of the ice crystal and liquid pore water, $\kappa_{cl} = (\mathbf{1}_T : \boldsymbol{b})$ is the reciprocal of curvature radius of the interface $\mathcal{I}^{cl}$.

In addition to the mechanical equilibrium in the interface $\mathcal{I}^{cl}$ (see Eq. (2)), the thermodynamic equilibrium of the interface $\mathcal{I}^{cl}$ between ice crystal and liquid pore water should also be obeyed (Coussy, 2011). With the assumption of hemispherical interface $\mathcal{I}^{cl}$ ($\kappa_{cl} = 2\cos\theta/r_{cr}$), according to the thermodynamic equilibrium and mechanical equilibrium of the interface $\mathcal{I}^{cl}$, the freezing temperature can be depressed by the capillary effect according to the following modified Gibbs–Thomson equation (Coussy, 2011):

$$\frac{2\gamma_{cl}\cos\theta}{r_{cr}} = \left(\frac{V_l}{V_c} - 1\right)(P^l - P_0) - S_m\delta T \tag{3}$$