



Numerical modeling of drying shrinkage deformation of cement-based composites by coupling multiscale structure model with 3D lattice analyses



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ARTICLE INFO

Article history:

Received 20 March 2016

Accepted 4 October 2016

Keywords:

Drying shrinkage

Water desorption

Multiscale model

Lattice analysis

Capillary pressure

ABSTRACT

This paper presents a multiscale model for the drying shrinkage deformation of cement-based composites by incorporating its corresponding multiscale computer-generated structure at different scales in a three-dimensional lattice model. Assuming effects of capillary tension and disjoining pressure are the reason for the drying deformation, water desorption in capillary pores within 100%-to-85% RH range and that in gel pores within 85%-to-50% RH range are investigated. Drying behaviors of C-S-H gels, cement paste and mortar are studied by gradual upscaling. Experimental results for cement paste and mortar are utilized for validation. Parameter-determination and parameter-passing associated with the multiscale model are discussed.

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1. Introduction

Drying shrinkage deformation can be a major cause of the deterioration of concrete structures and has been intensively investigated [1–19]. In the range of relative humidity (RH) that a typical concrete structure will experience, the driving forces of shrinkage are generally considered as capillary tension and disjoining pressure [10,19–23]. The macroscopically observed drying shrinkage deformation of concrete, in principle, is determined by the water existing in calcium-silicate-hydrate (C-S-H) and in the capillary pores of cement paste. For the purpose of exploring the drying nature of cement-based materials, knowledge of the water desorption processes in the nanostructure of C-S-H and in the microstructure of cement paste, of the deformation of C-S-H, of the deformation of cement paste is needed.

In simulation, for a microstructure-based approach, it is a conflict between computing the drying deformation of big size materials (i.e., concrete, on the order of magnitude millimeter to

meters) and incorporating the stimulus source at very small size (i.e., water pressure change in the pores on the order of magnitude nanometers). In order to solve this problem, multiscale models are proposed. Multiscale models aim to establish a relation between macroscopically observable phenomena and their finer-scale origin [24]. Based on the structure of materials in question at a respective observation scale, the physical/chemical/mechanical/hygro processes within the materials can be considered [25–30] and their effect on the macroscopic material performance can be obtained by means of appropriate upscaling schemes [24,31–36]. Combining continuum micromechanics with cement hydration models, Pichler et al. [24] have proposed a multiscale model to predict the autogenous-shrinkage deformation of cement-based materials. Combining three-dimensional lattice fracture model with material models of C-S-H and cement paste, Liu et al. [17] have developed a two-scale model to predict the drying shrinkage of cement paste for high humidity case. Nevertheless, rare modeling work is reported based on a systematic approach including water desorption processes in the nanoscopic and microscopic pores, the response of C-S-H gels and cement paste to the water desorption at different scales, and the consequent drying shrinkage deformation of cement-based composites. The goal of this paper is to investigate the above issues systematically.

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This paper presents a multiscale microstructure-based model to predict the drying shrinkage deformation of cement-based materials. The combined application of a multiscale material model and a three-dimensional (3D) lattice model makes it possible to study the drying behaviors of C-S-H gels, cement paste and mortar by gradual upscaling and by incorporating the contribution of capillary water, gel water as well as interlayer water. Assuming effects of capillary tension and disjoining pressure are the main reason for the drying deformation of cement-based materials, the water desorption in capillary pores within 100%-to-85% RH range and that in gel pores within 85%-to-50% RH range are investigated. Experimental results for the drying shrinkage of cement paste are utilized to validate the proposed model. The parameter-determination and the parameter-passing associated with the multiscale model are finally discussed.

2. Capillary pressure and disjoining pressure

In general agreement, changes in capillary pressure, disjoining pressure and the surface tension of solid particles are assumed as mechanisms governing drying shrinkage. Whether a particular mechanism is active is dependent on the internal relative humidity (RH) within the material.

- At high humidity (100%-to-85% RH), moisture loss occurs in capillary pores and gel pores remain full of water [10,37]. Effects of capillary pressure and disjoining pressure are active [19,20].
- At mid humidity (85%-to-45% RH), moisture loss occurs in gel pores and only a small amount of liquid water exists in capillary pores [17,37]. Effects of capillary pressure and disjoining pressure are still active [10,19,20].
- At low humidity (below about 40–45% RH), capillary menisci are not stable and the effect of capillary pressure is not present [20]. Effects of disjoining pressure and surface tension of solid particles are active [19–21].

Recently, Jennings et al. argued that the effect of surface tension of solid particles may below 20–25% RH [10,18]. Normally, the capillary pressure mechanism and the disjoining pressure mechanism are assumed to be predominant because the internal RH of a typical concrete structure will experience intermediate to high humidity [20]. Fig. 1 illustrates the geometrical presentation of disjoining pressure zone and capillary pressure zone in a liquid bridge between two spherical substrates. The disjoining pressure is active in areas of hindered adsorption, i.e. where the distances between the solid surfaces are smaller than two times the thickness of the free adsorbed water layer [21], and the rest of the water zone is the capillary pressure zone.

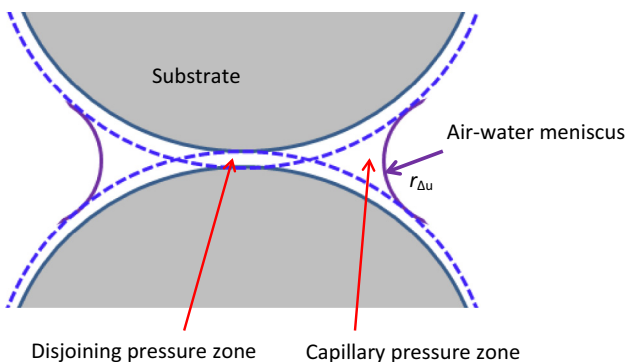


Fig. 1. Geometrical illustration of capillary adhesion and disjoining pressure zones.

Kelvin equation, given below, has been widely used in evaluating the capillary pressure and disjoining pressure [22],

$$p_{\text{atm}} - p_L = -\frac{RT}{\bar{V}_L} \ln h_R \quad (1)$$

where p_L is pressure in pore fluid, MPa; p_{atm} is the atmospheric pressure, MPa; \bar{V}_L is the molar volume of water, cm^3/mol ; R is the universal gas constant, $\text{J}/(\text{mol}\cdot\text{K})$; T is temperature, K ; h_R is the value of relative humidity. At above 45% RH, the Kelvin equation accounts for both the shrinkage stress associated with the surface tension and the disjoining pressure mechanisms [20]. The capillary pressure p_{cap} , reading as $p_{\text{cap}} = p_C - p_L$, can be written as the relation with the water-vapor menisci according to Laplace equation [15,22],

$$p_{\text{cap}} = \gamma_{LV} \kappa_{LV} \quad (2)$$

where γ_{LV} is the surface tension of the liquid/vapor interface, J/m^2 ; κ_{LV} is the curvature of the liquid/vapor interface, μm^{-1} ; p_C is the gas pressure, MPa. Once the gaseous equilibrium is achieved, the internal gaseous mixture is at the atmospheric pressure, $p_C = p_{\text{atm}}$. Based on a spherical meniscus, combining Eqs. (1) and (2), Kelvin-Laplace equation can be obtained, described as [22],

$$r_{\Delta u} = -\frac{2\gamma_{LV}}{(RT/\bar{V}_L) \ln h_R} \quad (3)$$

where $r_{\Delta u}$ represents the smallest pore access radius of the pore volume currently invaded by air, that is, pore radius threshold for drying at a specific h_R and T . For porous materials, if all the pores are highly connected and the air permeability is rather high, the assumption, $p_C = p_{\text{atm}}$, can hold. Otherwise, the gas pressure cannot be assumed to remain constantly equal to the atmospheric pressure, for example, for weakly permeable materials [38]. In this study, the assumption $p_C = p_{\text{atm}}$ is adopted. Take the atmospheric pressure p_{atm} equals to zero as reference, the stimulus stress for drying can be considered as a negative pressure of liquid water p_L , which can be obtained according to Kelvin equation. The validity of the Kelvin equation has been confirmed for several liquids and for menisci with radii as low as 4 nm by measuring capillary condensation [39–42]. Although the accuracy of the Kelvin equation to determine the critical pore radius is reduced when the interfacial radius is smaller than 4 nm, Eq. (3) has been extensively used in capturing capillary condensation [14,15]. The quantitative results may slightly deviate when the interfacial radius is smaller than 4 nm, however, the theory for the physical phenomenon should remain valid [43]. At 293.15 K, $R = 8.314 \text{ J}/(\text{mol}\cdot\text{K})$, $\bar{V}_L = 18.032 \text{ cm}^3/\text{mol}$ and $\gamma_{LV} = 0.072 \text{ J}/\text{m}^2$ are adopted [44]. Then, at 50% RH, the radius $r_{\Delta u}$ equals to 1.5 nm and at 85% RH, the radius $r_{\Delta u}$ equals to 6 nm.

The disjoining pressure between helium and glasses was measured by Sabisky and Anderson [45] with a balance under gravitational potential. However, it is still a challenge to quantify the absolute disjoining pressure in porous cement-based materials by direct measurements. Based on two assumptions, (a) the disjoining pressure is determined by the thickness of adsorption, and (b) the thickness of adsorption is determined by the ambient RH and temperature, Maruyama evaluated the disjoining pressure as a function of statistical thickness of absorbed water [46]. Nevertheless, it is difficult to quantify the statistical thickness of absorbed water at different RH. In this paper, using the Kelvin equation, the change in disjoining pressure can be quantified since the change in stress of the absorbed water must be the same as the change in stress for the evaporable water [20].

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