



Microstructure-based modelling of drying shrinkage and microcracking of cement paste at high relative humidity



Lin Liu^{a,b,*}, Xuecheng Wang^a, Huisu Chen^c, Chaojun Wan^d

^a College of Civil and Transportation Engineering, Hohai University, Nanjing 210098, China

^b Jiangsu Engineering Research Center of Crack Control in Concrete, Hohai University, Nanjing 210098, China

^c Jiangsu Key Laboratory of Construction Materials, School of Materials Science and Engineering, Southeast University, Nanjing 211189, China

^d College of Materials Science and Engineering, Chongqing University, Chongqing 400044, China

HIGHLIGHTS

- Water evaporation from capillary pores of cement paste is modeled.
- Micro-/nano-structure of cement paste are incorporated by two-scale modeling.
- Drying-induced shrinkage of cement paste is predicted by a 3D lattice approach.
- Internal microcracking with constrained boundary during drying is simulated.

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ABSTRACT

In order to comprehensively understand the drying behavior of cementitious materials, this paper presents a microstructure-based model to simulate the water evaporation process in capillary pores, the drying-induced deformation of cement paste with free boundary condition and the microcracking of cement paste under constraint. This model is applicable to high relative humidity ranges where the capillary pressure effect quantified by the Kelvin equation is the primary loading stimulus. Mainly two parts of modeling work are carried out. (1) From a microstructure model of cement paste HYMOSTRUC3D, the water evaporation in capillary pores is captured by a multi-step digitalization algorithm. (2) The drying-induced shrinkage deformation and internal microcracking of hardened cement paste with different boundary constraints are simulated by a 3D lattice fracture model. In order to reduce the computational cost, a two-scale modeling regime is employed where the microstructure of cement paste and the nanostructure of C-S-H are incorporated. Experimental test about free shrinkage of cement paste is utilized to validate the model. At last, the model is compared with poro-elastic-mechanical models, and is applied to study the influences of water-to-cement ratio and hydration time on the free shrinkage as well as the influence of constraints on the internal microcracking.

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1. Introduction

Most concrete structures in service are inevitably subjected to drying-induced shrinkage, and the drying shrinkage can be a major cause of deterioration of concrete structures [1,2]. When the internal humidity of cementitious materials decreases, i.e., exposed to low humidity environment or losing evaporable pore water through consumption in the hydration reaction, the material undergoes a drying process and shrinkage occurs. If the shrinkage

is externally or internally restrained, internal stress will develop and cracking may take place.

In order to reduce the shrinkage harm to concrete structures and to optimize materials design, influences of a number of factors on the drying shrinkage deformation, including relative humidity (RH), water/cement ratio (w/c), temperature, pore solution, aggregate size and amount, addition of supplementary materials and so on have been investigated by experiment [1–10]. From the experimental results, a number of numerical simulations have been performed to model the drying process of porous materials [9–15]. Among the simulations, a poromechanical approach is usually utilized to model the deformation of porous materials due to drying [11–13], because it can provide us a quantitative macroscopic approach to the physical mechanics occurring at the pore scale

* Corresponding author at: College of Civil and Transportation Engineering, Hohai University, Nanjing 210098, China.

E-mail address: liulin@hhu.edu.cn (L. Liu).

[12]. Nevertheless, the pore structure of porous materials, which is crucial to the drying process, is highly simplified in the poromechanical models using pore size distribution instead. As an alternative approach, computer models, especially microstructure-based models, can provide us an intuitive insight in the interaction between physical inferences and deformation or cracking capability [15–16]. So far, rare modeling work is performed to give an integrated description for the drying process and related consequences for cementitious materials based on a microstructure-based approach. Therefore, this paper aims to present a microstructure-based model to simulate the water evaporation process in capillary pores, the drying-induced deformation of cement paste with free boundary condition and the microcracking of cement paste under constraint. From the computational point of view, it would be of significance for fundamentally understanding the drying shrinkage problem of cement-based materials.

The principal mechanisms governing drying-induced shrinkage are changes in capillary pressure, changes in disjoining pressure and changes in the surface tension of solid particles with the changing RH [17–20]. At mid to high RH, capillary pressure and disjoining pressure are active. The division between mid and high RH is usually adopted as 85% RH [21]. From 100%-to-85% RH, capillary water in cement matrix can get empty according to a pore blocking mechanism. As the RH subsequently decreases, gel water in calcium-silicate-hydrate (C-S-H) can get empty. At low RH, i.e., below about 40%–50% RH, capillary menisci are not stable and the effect of capillary pressure is not present [19,21,22]. Then, the drying shrinkage is typically attributed to disjoining pressure and surface tension of solid particles [17,19,20].

Changes of capillary pressure and disjoining pressure can be calculated from Kelvin equation, given by [18],

$$p_{\text{atm}} - p_L = -\frac{RT}{V_L} \ln \frac{p_V}{p_{V_S}(T)} \quad (1)$$

where p_L is pressure in pore fluid, MPa; p_{atm} is the atmospheric pressure, MPa; 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 . p_V represents the partial pressure of water vapor, MPa; $p_{V_S}(T)$ represents the saturated pressure of water at a given temperature T , MPa. According to the definition of RH, that is the ratio of the partial pressure of water vapor p_V to the saturated vapor pressure of water $p_{V_S}(T)$ [18,19],

$$h_{\text{RK}} = \frac{p_V}{p_{V_S}(T)} \quad (2)$$

h_{RK} represents the value of relative humidity due to menisci formation in a pore. At gaseous equilibrium, the internal gas pressure in cementitious material is assumed to equal to the atmospheric pressure, i.e., $p_G = p_{\text{atm}}$, then Eq. (1) can be rewritten as,

$$p_G - p_L = -\frac{RT}{V_L} \ln h_{\text{RK}} \quad (3)$$

Using Eq. (3), the capillary pressure p_{cap} , or the disjoining pressure p_{dsj} , reading as,

$$p_{\text{cap}} = p_G - p_L \quad (4a)$$

$$p_{\text{dsj}} = p_G - p_L \quad (4b)$$

can be related to the RH. The disjoining pressure is active in the areas of hindered adsorption, where the distances between the solid surfaces are smaller than two times the thickness of the free adsorbed water layer [17], while the capillary pressure is active in the areas of water-filled pores whose size are larger than that. The accuracy of the Kelvin equation has been investigated intensively and its validity has been confirmed at high RH ranges

[23–25]. Since changes in the disjoining pressure with the changing RH are the same as capillary pressure does following Eq. (3), contribution of disjoining pressure to drying is classified as capillary pressure effect, for simplicity.

Laplace equation, given below, can provide the link between the capillary pressure and pore geometry,

$$p_{\text{cap}} = \gamma_{LV} \kappa_{LV} \quad (5)$$

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} . Based on a spherical meniscus, combining Eqs. (3)–(5), Kelvin-Laplace equation can be obtained, described as,

$$r_{\Delta u} = -\frac{2\gamma_{LV}}{(RT/V_L) \ln h_{\text{RK}}} \quad (6)$$

where $r_{\Delta u}$ represents the smallest pore access radius of the pore volume currently invaded by air at h_{RK} and T . Based on Eq. (6), the water-vapor menisci in capillary pores and capillary water evaporation can be configured.

Starting from moisture cured state, as RH decreases, capillary water in cement matrix start to get empty following the water evaporation rule, i.e., Eq. (6), and a pore blocking mechanism. The pore blocking phenomena is high dependent on the capillary pore structure because it is the channel of water evaporation. At the same time, effect of capillary pressure active in capillary pores and gel pores will result in contraction of the material. Therefore, all capillary pores, gel pores and the solid part of the cement paste are necessary in modeling of its drying behavior. In this study, in order to reduce the computational cost of a microstructure-based computer model, the above information is incorporated by a two-scale modeling regime where the microstructure of cement paste and the nanostructure of C-S-H are coupled.

From the drying mechanism and the two-scale material modeling, this paper presents a method to simulate the water evaporation process in capillary pores, the drying-induced deformation of cement paste with free boundary condition and the cracking of cement paste under constraint. First, the water evaporation in capillary pores is captured from the microstructure of cement paste by a multi-step digitalization algorithm. Second, the shrinkage of C-S-H gels are estimated through 3D lattice analyses on their nanostructures, those of low density (LD) and high density (HD) C-S-H are considered, respectively. Then, taking the water distribution in capillary pores and the shrinkage of C-S-H gels into account, the drying-induced shrinkage and microcracking of hardened cement paste with different boundary constraints are simulated by a lattice model. Simulation results about free shrinkage of cement paste are validated through experimental tests. In the discussion part, the predicted drying shrinkage deformation of cement paste is compared with those by poro-elastic-mechanical models, and the influences of water-to-cement ratio, hydration time and boundary constraint on the free shrinkage as well as the internal microcracking are investigated.

2. Modeling methodology

There are some assumptions are made before modeling: (1) Gaseous equilibrium in all pores is achieved, so that $p_G = p_{\text{atm}}$ can hold. (2) At microscopic scale, no RH gradient exists in the microstructure of cement paste with a length of tens to a hundred micrometers. (3) High RH range (80% RH above) is considered. The initial status of cement pastes is assumed to be water-saturated. Capillary water in cement paste can get empty with the decreasing RH, while the gel water remains full. (4) Capillary pressure effect is assumed as the primary loading stimulus and active in capillary pores and gel pores.

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