Construction and Building Materials 120 (2016) 494–503

Contents lists available at ScienceDirect

Construction and Building Materials

journal homepage: www.elsevier.com/locate/conbuildmat

A three-dimensional multi-scale method to simulate the ion transport behavior of cement-based materials

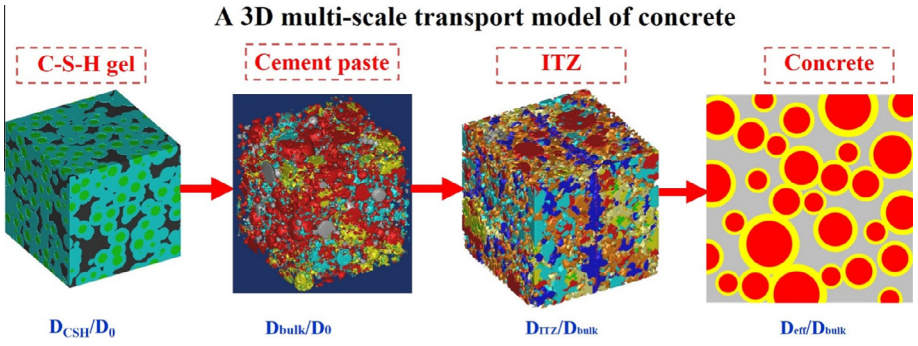
Zhiyong Liu [a,b,c,*], Weiwei Chen [a,b], Yunsheng Zhang [d], Henglin Lv [a]

[a] Jiangsu Key Laboratory of Environmental Impact and Structural Safety in Engineering, China University of Mining and Technology, Xuzhou 221116, China
[b] State Key Laboratory of Geomechanics & Deep Underground Engineering, China University of Mining and Technology, Xuzhou 221116, China
[c] JiangSu Collaborative Innovation Center for Building Energy Saving and Construct Technology, Xuzhou 221116, China
[d] Jiangsu Key Laboratory for Construction Materials, Southeast University, Nanjing 211189, China

HIGHLIGHTS

- 3D microstructure of C-S-H with micro and macro scales is generated.
- ITZ of single flat plate aggregate is established.
- A multi-scale transport model ranging from nano-scale, micro-scale, to macro-scale of concrete is proposed.

GRAPHICAL ABSTRACT



ARTICLE INFO

Article history:
Received 5 April 2016
Received in revised form 16 May 2016
Accepted 19 May 2016
Available online 26 May 2016

Keywords:
Cement-based materials
Transport
Multi-scale
Three-dimensional

ABSTRACT

The formation process of microstructures in cement pastes was first simulated with a numerical model. The simulated masses of the $Ca(OH)_2$ and C-S-H phases were verified by measuring values with thermogravimetry-differential scanning calorimetry (TG-DSC) and XRD-Rietveld analysis. Then, the main transport paths for corrosive media, including nano-scale C-S-H gel pores, micro-scale capillary pores and the interface transition zone, were extracted, and the corresponding effective transport coefficients were determined. Finally, a multi-scale transport model ranging from the nano-scale through the micro-scale and to the macro-scale of concrete was established based on the porous media mechanics and multi-scale method, combined with numerical calculation and 3D visualization. This model will help to design and predict the service life of concrete structures.

1. Introduction

Chloride ingress into concrete causes reinforcement corrosion, and the diffusion coefficient of chloride ions primarily affects the service life and durability of concrete [1,2]. A series of experimental tests have been developed during the past several decades to investigate the diffusion behaviors of chloride ions in cement-based materials [3–5]. For example, the diffusion coefficients of chloride have been measured by rapid chloride penetration tests [1,6], non-steady-state migration [7], steady-state conductivity methods [8], hydro-abrasion test [9]. However, these tests are very time consuming, and the experimental data have significant variability due to differences in measurement and sample preparation.

* Corresponding author at: Jiangsu Key Laboratory of Environmental Impact and Structural Safety in Engineering, China University of Mining and Technology, Xuzhou 221116, China.
E-mail address: liuzhiyong0728@163.com (Z. Liu).

http://dx.doi.org/10.1016/j.conbuildmat.2016.05.121
0950-0618/

To overcome the shortcomings of the experiments, the transport properties can also be predicted and analyzed using empirical equations, analytical models and numerical simulations. Papadakis VG et al. considered the effect on ambient relative humidity (RH), the diffusivity is given by an empirical equation [10]. Oh BH et al. proposed a simple analytic model that can predict realistically the diffusivities of concrete and mortar [11]. Huang Q et al. presented a numerical approach for predicting moisture transport in concrete based on pore size distribution represented by a multi-Rayleigh–Ritz model that includes gel pores, small and large capillaries, and microcracks [12]. However, predicting ion diffusion is a great challenge because concrete has a complex microstructure and exhibits composite behaviors over many length scales [13]. A large range of length scales from nanometer-sized pores to millimeter-sized aggregates for modeling concrete require a multi-scale approach [14,15] to predict the chloride ion diffusion. The ion diffusion properties computed at a micrometer scale are fed into the model constructed at the next higher scale, such as the millimeter scale.

In this study, the micro and macro of C-S-H gel model are constructed and the information of pore structure is acquired in nanometer scale. Two separate models are developed for the cement paste surrounding a single aggregate (micrometer scale) and a representative volume of concrete (millimeter scale). The C-S-H gel diffusivity coefficient at a nanometer scale is incorporated at the micrometer scale and the millimeter scale. Therefore, seven orders of magnitude of the length scale (10^{-9}–10^{-2} m) are contained in this multi-scale modeling method. The effective diffusivity of concrete is finally computed and compared to experimental results for validation.

2. Multi-scale modeling method

2.1. Nanometer-scale model

Based on the experimental results of transmission electron microscopy (TEM), Bentz [16] divided C-S-H into two scales (micro and macro). The micro scale is a small part of the macro-scale units, and their relationship is shown in Fig. 1. Powers [17] has reported that the total porosity of C-S-H is 28%. According to the isotherm absorption experiment, the porosity of the micro-scale and macro-scale are 22.3% and 7.6%, respectively. The parameters of the micro and macro models are listed in Table 1.

According to the parameters in Table 1, the three-dimensional structure of C-S-H is established. In this model, C-S-H particles as a hard core are assumed to spherical. The outside of the hard core is surrounded by a layer to allow overlapping concentric soft shells. For simplicity, all of the C-S-H particles and the soft shells are assumed to be the same size. Using a periodic boundary, the particles are randomly placed into a cube cell. The corresponding porosity of the C-S-H microstructure can then be acquired. The 2D and 3D images of C-S-H gel for micro- and macro-scale are shown in Fig. 2. The porosity of the micro-scale is significantly larger than that of the macro-scale. The average pore size of micro and macro are 3.69 nm and 14.17 nm, respectively.

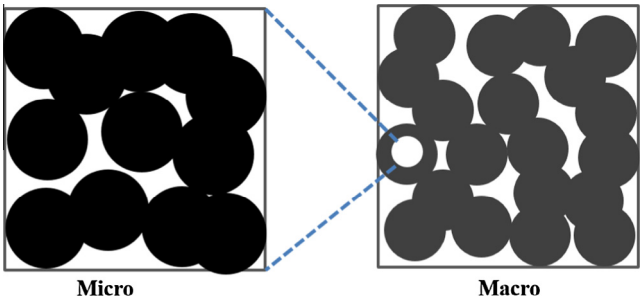


Fig. 1. Relationship between micro and macro levels.

For cement-based composite materials, the relative diffusion coefficient is an important parameter to study its transport behavior. According to the Nernst-Einstein equation, the relative diffusion coefficient (D/D_0) is equal to the relative electrical conductivity (σ/σ_0). Based on the C-S-H gel of the micro and macro models, the electrical analog method can be used to calculate the relative diffusion coefficient of the two dimensions.

First, the continuous matrix micro and macro models are divided into a three-dimensional lattice network; then, the discretization of the model is converted into an electrical network; and finally, the conjugate gradient method is adopted to calculate the relative conductivity (diffusion coefficient) of porous materials. The discrete model has three phases, as shown in Fig. 3. After obtaining the digital image, a pixel size of the electrode is pasted on the back of the digital unit and a node is set in the middle of each pixel, thus forming a network of nodes. The conductance (Σ_{ij}) of two adjacent pixels (i, j) can be used in a series model:

$$\Sigma_{ij} = 1/(1/\Sigma_i + \Sigma_j) \tag{1}$$

$$\Sigma_i = \sigma_i \times d^2/(0.5d) = 2\sigma_i d \tag{2}$$

where Σ_i represents the conductance of a half pixel unit i and d is the length of a pixel unit. If pixels i and j are pore phase, $\sigma_i = \sigma_j = 1$ and $\Sigma_{ij} = 1$. If at least one of the pixels i and j is a solid phase, the conductivity of the solid phase is zero, so $\Sigma_{ij} = 0$.

According to the Eqs. (1) and (2), the conductance of each node is calculated in Fig. 3. Because the hard core and soft shell of the C-S-H model cannot belong to conductive solid phases, the conductance of the node for the no connecting lines, the dotted lines and the thin lines are zero in the figure. The conductance of the thick solid lines is d. The arrows indicate the connection between electrodes and conductors. If connecting pores to each other, the conductivity is $2d$; if connecting solid phases to each other, the conductivity is 0.

After the conductance of the C-S-H gel network structure is generated, the conjugate gradient relaxation algorithm is employed to calculate the conductivity of the lattice network. Applying a potential difference, the model can test the voltage of each node, and then determine the current and conductance. Voltages of 1 and 0 are applied in the lattice model on both ends, respectively, in line with the linear interpolation between nodes. The node voltage is constantly updated until the sum of current flowing into a node is equal to that flowing out from the node.

To save computation time and stabilize the calculation results, the effects of the different calculation steps in the conjugate gradient algorithm on the macro-scale relative diffusion coefficients are analyzed. From Fig. 4, the X, Y, and Z direction results are not the same, showing that the calculated relative diffusion coefficients of the electrical simulation exhibit 3D structure anisotropy. The

Table 1
Parameters of micro and macro levels.

Scale	Length size	Pixel resolution	Particle diameter	Size of hard core	Size of soft shell	Number of particles	Porosity
Micro	25 nm	0.125 nm	5 nm	3.7 nm	1.3 nm	212	22.3%
Macro	250 nm	1.25 nm	40 nm	22 nm	18 nm	675	7.63%