Construction and Building Materials 170 (2018) 326–346

Contents lists available at ScienceDirect

Construction and Building Materials

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

The effect of microscopic cracks on chloride diffusivity of recycled aggregate concrete

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HIGHLIGHTS

- A novel stochastic numerical method to investigate the effect of cracks on diffusivity of RAC.
- Two-dimensional fictitious multi-phase RAC models are randomly generated.
- Effective homogenized ion diffusion coefficients of RAC models are computed using RVE approach.
- Microscopic defect number, direction, and length might have significant influence.

ARTICLE INFO

Article history:
Received 8 September 2017
Received in revised form 1 March 2018
Accepted 5 March 2018

Keywords:
RAC
Microscopic cracks
Chloride diffusivity
Stochastic
Homogenization

ABSTRACT

This study proposes a novel stochastic numerical method to investigate the effect of microscopic cracks on chloride diffusivity of recycled aggregate concrete. First of all, two-dimensional fictitious multi-phase recycled aggregate concrete (RAC) models are randomly generated. The fictitious RAC models consist of microscopic cracks in addition to natural aggregate, old interfacial transition zones (ITZs), old mortar, new ITZs, and new mortar. Next, effective homogenized ion diffusion coefficients of RAC models are computed using representative volume element (RVE) approach, after the size of RVE is determined by convergence analysis. Then a series of Monte Carlo simulations are made to explore the link between randomly distribution of microscopic cracks and the effective homogenized ion diffusivity. Finally, the numerical experimental results indicate that microscopic defect number, direction, and length might have significant influence on the effective homogenized ion diffusion parameter of RAC. In addition, this study investigates material property uncertainties of ITZs and mortar on the global chloride diffusivity of RAC. Final results demonstrate that effects from material property uncertainties of ITZs and mortar might be negligible.

1. Introduction

The last two decades have seen growing importance placed on research in multiscale numerical theory of the diffusivity of concrete [1–6]. Multi-scale problem that is commonly used in some analysis tools, for example, the average method, the methods of homogeneous, the renormalization group method, the asymptotic matching method, etc., have been adopted in the analysis and research of the recycled concrete chloride ion diffusion. Some scholars explicitly use the multi-phase asymptotic analysis model. When the macro empirical model is not enough, some scholars use numerical methods to obtain the macroscopic behavior of complex systems. To solve local singularities, losses and other problems, some scholars use numerical methods to combine macro and micro models. In addition, some scholars have studied the differential equations with multiscale coefficients, slow and fast dynamic problems, and other special problems.

The multi-scale model relates to the problem of the cross-level fundamental unity and the coupling mechanism which corresponds to the coupling strength [7–10]. Therefore, the establishment and selection of theoretical and numerical algorithms is a complex problem. Is related to the low limit of nanoscale quantum mechanics, and the atomic scale associated with upper limit nanoscale science - molecular dynamics and Monte Carlo method, classical mechanics also relate to the macro scale, density functional theory, and the parameters of the classical theory of corresponding analytical method, can form processing small scale LAN effect theory. In recent years, some scholars in the condensed matter system have developed the hierarchical coupling method and the cross-layered collaborative coupling algorithm. In terms of the integrity of theoretical processing and the validity of numerical

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https://doi.org/10.1016/j.conbuildmat.2018.03.045
0950-0618/

calculation, these studies reflect the important progress of multi-scale computation.

Based on the general point of view, the problem of small scale effect or macro-scale continuous medium must be dealt with in different ways in terms of the level and nature of physical property [11–13]. The same method is difficult to solve the multi-scale problem. In terms of multi-scale problems, hybrid algorithm, wavelet method, multi-grid technique and multi-level finite element method are presented to solve the problem of multiple decomposition. The hybrid algorithm is based on quantum mechanics, atomic simulation, and finite element. The characteristic of wavelet method is to show the information of discrete on different scales, which can be shown on the average of large scale, which partly reflects the multi-scale coupling. The finite element method provides an effective and flexible numerical calculation technique for the model unknown function. The multi-grid method is characterized by the representation of the whole function at the fine level and provides an effective way to solve the multi-scale problem.

Main methodologies in these multiscale models were classified as the three approaches, the N-layered spherical mixture method, the hybrid lattice Boltzmann finite element method, and the comprehensive probabilistic method. Sun et al. [14,15] calculated the homogenized diffusion coefficient of chloride ion in cement-based materials using N-layered spherical mixture model. Zhang et al. [16,17] presented the algorithms and implementation of hybrid lattice Boltzmann-finite element method that combines the advantage of lattice Boltzmann method and finite element method to estimate the chloride diffusivity in cement materials. Bastidas-Arteaga et al. [18] proposed a comprehensive probabilistic model of chloride ingress in unsaturated cement materials. The uncertainties related to the problem were also considered using random variables to represent material properties and stochastic processes.

The continuing improvements in the multiscale numerical methods of diffusivity of concrete have led to many new and fascinating extension to chloride diffusivity prediction of recycled aggregate concrete. For example, Xiao et al. [19] proposed a mesoscopic five-phase model to study the effect of recycled aggregate on the chloride diffusion in recycled aggregate concrete considering the old and new ITZs. Ying et al. [20,21] proposed a five-phase composite sphere model for the matrix in recycled aggregate concrete for chloride diffusivity. The effects of recycled coarse aggregate distribution on chloride diffusion of the RAC model were investigated with different aggregate replacement ratios.

As matter of fact, the probabilistic method has been widely applied in fiber reinforced composite including stochastic interface defects. For example, Kaminski et al. [22–24] presented a numerical method for a homogenization problem of random elastic composites with stochastic interface defects. Then, the method was extended to explore material sensitivity (Kaminski et al. [25–27]), fatigue behavior (Kaminski et al. [28]), semi-elliptical random interface defects (Kaminski et al. [29]), and stochastic aging effect (Kaminski et al. [30,31]). In addition, Sakata et al. [32] presented three-dimensional stochastic analysis using a perturbation method for elastic properties of composite material considering microscopic uncertainty. Then, the stochastic homogenization method was extended to investigate elastic properties of fiber reinforced composites (Sakata et al. [33]), and microscopic failure probability (Sakata et al. [34]). Moreover, Xu [35] developed a stochastic finite element method to resolve scale-coupling elliptic problems, based on formulations of a stochastic variational approach and scale-bridging multiscale shape functions. Furthermore, Hou and Liu [36] introduced a new concept of sparsity for the stochastic elliptic operator to reflect the compactness of its inverse operator and allows for spatially heterogeneous structure.

Because the mechanical properties of recycled concrete are lower than that of ordinary concrete, it is necessary to study the mechanical properties of recycled concrete. Some scholars used the chemical slurry to strengthen the recycled aggregate, and put forward the feasibility of high strengthening of recycled aggregate concrete. Some scholars have taken to reduce the water cement ratio and high efficiency water reducing agent, adding proper amount of fly ash to strengthening of recycled aggregates. They found that the lower water/cement ratio can make the recycled concrete interface transition zone much closer. In addition, some studies have found that the secondary agitation process can make the interfacial transition zone structure denser, improve the strength of recycled concrete, and reduce the dispersion of intensity. There is also a new type of stirring process, which can be used to increase the mechanical properties of recycled concrete by wrapping a layer of volcanic ash on the surface of the recycled aggregate before pouring. Also, the mechanical properties of recycled aggregate can be improved by microwave heating technology.

Interfacial transition zone is a narrow area between natural aggregate and cement mortar in concrete. Its performance is related to many factors, such as cement material type, mix ratio, hydration age, stirring process and shape of aggregate type. Compared with ordinary concrete, the microstructure of recycled concrete is much more complex. It contains various mortar and interfacial transition zones. Some scholars have applied nanomechanical testing technology to directly measure the nanomechanical properties of the interface transition zone in cement concrete, including elastic modulus and indentation hardness. In general, nano indentation technology and microhardness testing technology are similar. But nano indentation technology has higher resolution, by which the local mechanical property of smaller area can be obtained. In addition, some study compared nano mechanical properties of interface transition zone in the different mixing processes, to provide foundation for improvement and modification of recycled aggregate concrete.

Unfortunately, although the recycled aggregate concrete is full of microscopic interface defects and is highly heterogeneous, little literature has been published on stochastic homogenization or heterogeneous multiscale finite element analyses for chloride diffusivity of RAC. Only a few isolated recent efforts have continued to investigate the effect of microscopic uncertainty on the global chloride diffusivity in the RAC model. Therefore, the central purpose of the research was to examine the effect of microscopic uncertainty on the homogenized chloride diffusivity in the RAC model.

This study proposes a novel stochastic numerical method to investigate the effect of microscopic cracks on chloride diffusivity of recycled aggregate concrete. First of all, two- dimensional fictitious multi-phase recycled aggregate concrete (RAC) models are randomly generated. The fictitious RAC models consist of microscopic cracks in addition to natural aggregate, old interfacial transition zones (ITZs), old mortar, new ITZs, and new mortar. Next, effective homogenized ion diffusion coefficients of RAC models are computed using representative volume element (RVE) approach, after the size of RVE is determined by convergence analysis. Then a series of Monte Carlo simulations are made to explore the link between randomly distribution of microscopic cracks and the effective homogenized ion diffusivity.

In general, this study focuses on discussion of the following research questions:

1. Does microscopic crack number have influenced on the effective homogenized chloride diffusivity of RAC?
2. Does microscopic crack direction have influenced on the effective homogenized chloride diffusivity of RAC?