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Multiscale digital-image driven stochastic finite element modeling of chloride diffusion in recycled aggregate concrete

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HIGHLIGHTS

- We simulate recycled aggregate concrete diffusivity using a novel multiscale stochastic method.
- The thickness of new ITZ greatly affects variation of RAC chloride diffusivity.
- The shape and size of recycled aggregate considerably affects variation of RAC chloride diffusivity.
- The proposed digital image kernel is very sensitive about noise.

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ABSTRACT

For estimation of the durability of recycled aggregate concrete (RAC) in chloride-rich environment, it is valuable to investigate the chloride diffusivity in RAC. Because RAC is highly heterogenous, an ideal five-phase model was designated as the representative research object of RAC in this paper. To investigate the effect of micro-scale randomness on the *meso*-scale chloride diffusivity in RAC, this paper developed a multiscale digital-image driven stochastic method, in which the digital-image covariance kernel was used in the Karhunen-Loeve expansion to generate basis functions for the model. The proposed method was at the first time used to analyze chloride ion diffusion in RAC. Through a couple of numerical experiments, it is indicated that the effects of aggregate shape, aggregate size and the thickness of interfacial transition zones (ITZs) are considerable on the coefficient of variation of chloride diffusivity in RAC. It is also found that the digital image kernel is more sensitive about noise than other standard covariance kernels.

1. Introduction

Global attention was paid on the research of the durability of reinforced concrete structures because of its significant influence on concrete structures. Chloride diffusivity was especially necessary to be determined because it had significant effect on durability of concrete structures in a marine or high salinity environment [42]. Sun et al. [27] developed a multi-scale model which treated concrete as four-phase composite materials consisting of matrix phase, aggregate phase, interfacial transition zone (ITZ) and their homogenization phase. Zheng et al. [43] examined the influence of the aggregate-cement paste interfacial transition zone on the steady-state chloride diffusivity of mortars and concretes using a semi-empirical, three-phase composite sphere model. Then, he developed an effective medium method to predict the chloride diffusivity in concrete [44]. Li et al. [18] treated concrete as a heterogeneous material composed of cement paste and aggregate, and assumed that chloride diffusivity took place only in the cement paste phase. Zhang et al. [39,40] utilized the multiscale lattice Boltzmann-finite element modeling method to investigate chloride diffusivity in cementitious materials. Also, there were some researchers focusing on influence of cracking on chloride diffusivity [8,6,36].

During development of civilization, a shortage of natural resources was showing up. In the construction filed, the technology of recycled aggregate concrete (RAC) was very important for environmental protection and sustainable development [37,38]. The properties of chloride diffusivity of recycled aggregate concrete (RAC) were more complex than that of natural aggregate concrete (NAC). It was acknowledged that recycled aggregates were always attached with old cement pastes on the surface which resulted in that RAC was more heterogenous than NAC. Therefore, the microstructure of ITZ in RAC was of more uncertainties, different

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Nomenclature

A	the stochastic basis function	ε	the error of the approximation of Karhunen-Loeve expansion
$a(,)$	a bilinear variational form	ζ	the parameter related micro-scale Y to *meso*-scale X
C_{ij}	the covariance matrix	ω	the stochastic variable
D	the chloride diffusivity of hardened cement paste	Θ	the orthogonal discrete random series
D_a	the chloride diffusivity of the aggregates	Λ	the Hilbert space
D_p	the chloride diffusivity in the pore solution	λ_i	eigenvalues
$\mathbf{D}$	the chloride diffusivity coefficient tensor	μ_i	the mean of Θ_i
$\mathbf{D}^{\zeta}$	the chloride diffusivity coefficient tensor at micro-scale	ξ	the variational chloride ion concentration
$\mathbf{D}^{(\mathrm{eff})}$	the homogenized diffusivity of the recycled aggregate concrete model	$\rho_{\mathrm{w/c}}$	the water-to-cement ratio
f_p	the porosity of cement paste	σ_i	the standard deviation of Θ_i
H	the stochastic series	Φ	the chloride ion concentration
$L()$	a linear variational form	Φ_i	eigenvectors
$\bar{q}_i, \bar{\mathbf{q}}$	the interfacial conditions between two phases		
x, X	the *meso*-scale coordinates		
y, Y	the micro-scale coordinates		

from that in NAC [33]. There have been significant advances in experimental and theoretical studies about the subject of chloride diffusivity in RAC in recent years. Most researches regarded experiment as the main research method, but the results of different experiments were of highly discrete distribution. Thus, the theoretical analysis of RAC was increasingly important. For example, Wang et al. [28] established a three-part model to analyze the chloride coefficient of the new ITZ in RAC. Xiao et al. [34] and Ying et al. [37,38] developed a model in *meso*-scope as a five-phase composite material to investigate the chloride diffusivity in RAC. In general, it was reasonable to treat RAC as microscopic heterogeneous materials to obtain a better understanding of the details of chloride ion diffusion in RAC.

In order to reveal the influence of microscopic uncertainties on the chloride diffusivity of RAC, this paper developed a simplified ideal recycled aggregate concrete model rather than develop a real complex RAC model. Researchers have made efforts to examine properties of RAC using the ideal aggregate concrete model. For example, Xiao et al. [31,32] conducted experimental and analytical investigations of the simplified concrete model containing nine aggregate types to study stress distribution and failure mechanism of RAC under uniaxial compressive loading.

On the other hand, it was necessary to establish a multiscale method to investigate the chloride diffusivity of recycled aggregate concrete for the sake of efficiency. The multiscale finite element methods (MsFEMs) were well developed in the pioneering works of Babuska and Osborn [2] and Babuska et al. [3]. In these papers, the authors suggested the use of multiscale basis functions to solve elliptic equation with a multiscale coefficient in one-dimensional field. This approach was extended in the work of Hou and Wu [10] to general heterogeneous materials. They generated an oversampling technique to improve the sub grid capturing errors. Nowadays, there have been many multiscale numerical methods developed to capture the multiscale structure of the solution via localized basis functions, including generalized finite element methods [1], homogenization approaches [23,14], equation-free computations [22,21], variational multiscale methods [20,13], heterogeneous multiscale methods [29], mixed multiscale finite element methods [19,12,35], and so on. The methods based on the homogenization theory have been successfully applied to the problems on heterogeneous materials.

Homogenization was one of the most effective mathematical tools for modeling and multi-component materials and structures. The method was first used for linear elastic and isotropic composite components. Kamiński et al. [15] put forward a formulation for a random composite with stochastic interface defects using the multiscale homogenization method. Then this method was extended to investigate sensitivity of periodic fiber-reinforced composites [16] and Gaussian uncertainty in material parameters [17]. Sakata et al. [24] proposed a perturbation-based homogenization method to investigate the influence of microscopic uncertainty on the elastic properties of an inhomogeneous material. Later, he applied the method to minimize the stochastic variation of homogenized elastic properties and a thermoelastic problem of unidirectional fiber-reinforced composites. In addition, Hou and Liu [9] introduced a new concept of sparsity for the stochastic elliptic operator, which reflected the compactness of its inverse operator in the stochastic direction and allowed for spatially heterogeneous stochastic structure.

Data-driven method was proposed in the computational mechanic field and applied for data-oriented program design [11]. In 1980s, the theory of dynamic data driven application system has been developed. Then it was involved in radiation transport, which enhanced the application of the models especially in cases where measurements were difficult to perform. Cheng et al. [4], Darema [5], and Zhang et al. [41] proposed a multiscale data-driven driven stochastic method for elliptic partial differential equations with random coefficients. Although the research on data-driven method was not as abundant as that of other available control theory, it attracted much attention because of its excellent performance to analyze complicate systems.

To investigate the effect of micro-scale randomness on the *meso*-scale chloride diffusivity in RAC, this paper developed a multiscale digital-image driven stochastic method, in which the digital-image covariance kernel was used in the Karhunen-Loeve expansion to generate basis functions for the model. This was the first time that the proposed method was used to analyze chloride ion diffusion in RAC. The main problems discussed in this paper were as follows:

- Is the proposed method feasible for chloride diffusion analysis in RAC?
- How does the error of mean chloride concentration change during data-driven processing?
- How does the shape of recycled aggregate affect the coefficient of variation of chloride diffusivity in the RAC model?
- How does the thickness of new ITZ affect the coefficient of variation of chloride diffusivity in the RAC model?
- How does the size of recycled aggregate affect the coefficient of variation of chloride diffusivity in the RAC model?