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Computational homogenization of effective permeability in three-phase mesoscale concrete

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HIGHLIGHTS

- 3D concrete mesostructure composed of three phases was modeled.
- Extensive Monte Carlo simulations for permeability test were realized and conducted.
- Effects of various mesostructural parameters on concrete permeability were investigated.
- RVE size regarding concrete permeability was evaluated by computational homogenization.

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ABSTRACT

Concrete is modeled on the mesoscale as a heterogeneous three-phase composite consisting of mortar, aggregates and the interfacial transition zone (ITZ). By exerting a steady state flow in the concrete sample, the effective permeability is estimated using finite element method (FEM). Extensive Monte Carlo (MC) simulations for more than 1000 concrete samples are carried out. The effects of the mesostructural parameters (i.e., the shape, gradation and volume fraction of aggregates and the thickness and permeability of ITZ) on the permeability of concrete are comprehensively investigated. For a specific set of mesostructural parameters, the size of the representative volume element (RVE) for concrete permeability is suggested in terms of the expected errors by numerical and statistical analysis. It shows that computational homogenization for estimating the effective permeability of concrete in three dimensions (3D) is absolutely necessary since the two dimensional (2D) results are less representative.

1. Introduction

In the design of dams and other large hydraulic structures, the rate at which water passes through concrete that is subjected to relatively high hydraulic pressure, i.e., water permeability, has long been recognized as a significant parameter for seepage analysis [1–3]. Permeability is also one of the most important transport properties influencing the durability and serviceability of concrete structures, since many durability problems (e.g., steel corrosion, sulfate or chloride attack, freezing-thawing cycles, abrasion and cavitations) are water-related [4–6]. The growing awareness of the role that permeability plays in the development of service life prediction models and optimum material design has led to the need for practical ways to quickly assess the permeability of concrete.

Laboratory-based tests have been conducted for many years to measure concrete permeability. It is widely recognized that direct experimental measurement of water permeability usually encounters practical difficulties for concrete due to its low permeability and the complicated conditions of testing methods [7,8]. Since concrete possesses a highly complex mesostructure composed of mortar (or cement paste), aggregates and ITZ between them, its transport properties are influenced by many interacting parameters related to the mesoscopic compositions which are difficultly identified by physical experiments [9,10]. Therefore, it would be extremely helpful to predict the transport properties of concrete based on its mesostructure, either with analytical or numerical models. Traditional close-form models available focusing on the mixture proportion like the Parallel model, the Series model, the Maxwell-Eucken (ME) model and the Effective Medium Theory (EMT) model reviewed in literature [11], are restricted to simple geometrical arrangements and fail to reveal the complicated transport behavior of concrete [12]. Over the past decade, with the advantages of repeatability and efficiency, numerical modeling

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emerges as a promising way for the study of the composite behavior of concrete with mesostructure. Many efforts have been made to explore the macroscopic transport properties of heterogeneous concrete, such as capillary absorption, diffusivity and permeability [13–17].

The influence of the mesoscopic compositions on the properties of concrete is strongly sensitive when the sampling volume size is comparable to that of aggregates. To estimate the material property of such a random heterogeneous material like concrete convincingly, sample size need to be large enough to guarantee statistical representativeness [18]. For this purpose, the concept of representative volume element (RVE) is generally introduced for computational homogenization of the effective properties [9,19,20]. As the volume size gets larger than RVE, the influence of the mesoscopic compositions on the properties of concrete weakens considerably and it could be assumed that the composite material is homogeneous in a statistical sense. Although the RVE on the mechanical properties of concrete has been investigated extensively, yet only a few of the studies on the size effect in modeling transport process are reported insofar.

Recently, some useful contributions have been made to determine the RVE from the perspective of transport properties by numerical simulation. For example, Keskin et al. [21] use a probabilistic model for 2D aggregate particles to evaluate the diffusivity of mortar and identify the smallest size needed for reliable estimations. Zhou and Li [22] conduct a numerical and statistical analysis of concrete permeability with a three-phase model in 2D. Nilenius et al. [23,24] study the effective moisture and chloride diffusivity coefficients in three-phase mesoscale concrete by computational homogenization. However, these simulations are carried out either in the case of 2D or using a composite sphere model in 3D, which might be less representative and insufficient for resembling the real concrete. Attributable to the extreme complexity of concrete material, these computer models still lack the required level of detail for taking into account the influential factors derived from its internal constituents, especially ITZ which is widely recognized as the zone of weakness in terms of fluid permeation. In order to gain a better knowledge of the RVE with regard to effective permeability of concrete, a realistic and sophisticated simulation of its mesostructure is urgently required.

In this paper, an investigation into the RVE of concrete for a rational estimation of its effective permeability via numerical simulation is presented. The exquisite model of concrete with a 3D mesostructure is generated, which is realized as three-phase composite material comprising of coarse aggregates, mortar matrix and ITZ. A steady state flow in the mesostructure of concrete can be implemented for investigating the water transport behavior and assessing its permeability using FEM. With Monte Carlo (MC) simulations, numerical studies on various factors influencing the permeability of concrete, such as the shape, gradation and volume fraction of aggregates and the transport property of ITZ, have been carried out to understand their impacts comprehensively. Subsequently, computational homogenization using the three-phase composite model is undertaken to determine the RVE size of permeability.

2. The three-phase mesoscale model

2.1. Generation of geometrical models

In the mesoscopic study, the 3D random aggregate structure (RAS) is first established for FE modeling. The geometrical model is the same as aforementioned: a three-phase composite consisting of homogeneous mortar matrix, randomly distributed coarse aggregates and ITZ of uniform thickness. The key factors for such a RAS resembling real concrete are the coarse aggregate configuration parameters, i.e., the size and spatial distribution, volume fraction and shape characteristic [13,25,26].

The size distribution of aggregates plays an important role in concrete mixture design, which affects the main properties of concrete such as workability of concrete mix, mechanical strength, permeability and durability [27,28]. In practice, concrete is most designed following Fuller curve [18,29] which is defined by

$$P(D) = 100\sqrt{D/D_{\max}} \tag{1}$$

where $P(D)$ is the cumulative percentage passing a sieve with aperture diameter D (L), and $D_{\max}$ (L) is the maximum size of the aggregate particles.

As one of the main constituents, coarse aggregates usually occupy around 0.4 of the concrete volume, which have proven to be an important influential factor on the overall transport properties of concrete [30–32]. Particles in various shapes are employed for modeling the aggregates, i.e., spherical or elliptical particles for gravel aggregates and convex polyhedral particles for crushed ones. These different shaped aggregates according to prescribed volume fractions and a specific size distribution (e.g., Fuller curve) are then randomly packed into a target cubic or cylindrical container for concrete samples, with the efficient approach of "occupation and removal method" [33,34]. 3D cubic geometrical models are generated in this study, with the detailed procedure described in our previous study [25]. Fig. 1 shows five typical models with particles of spherical shape in different sample sizes, L_s (L). Fig. 2 shows three models sized by $L_s = 150$ mm, containing spherical, elliptical and polyhedral shaped aggregates, respectively. In all these samples, the sizes of aggregates are scaling from $D_{\min} = 5$ mm to $D_{\max} = 40$ mm obeying Fuller curve and the aggregate volume fraction, f_{agg}, is fixed as 0.4.

2.2. Development of FE model

2.2.1. Governing equation

Suppose that the permeation of water in perfectly saturated porous medium obeys Darcy's law, which allows for the flow process driven by pressure gradient. Combining the continuity equation for incompressible and steady flow, water transport in concrete under the assumption that concrete skeleton is rigid, is governed by the following partial differential equation [1]:

$$\nabla(k \cdot \nabla\phi) = 0 \tag{2}$$

where k ($\mathrm{L\,T^{-1}}$) represents the permeability coefficient, ϕ (L) is the hydraulic potential and ∇ ($\mathrm{L^{-1}}$) is the spatial gradient operator. Eq. (2) is subject to appropriate boundary conditions:

$$\phi|_{\Gamma_1} = \phi_0 \text{ (first type)} \tag{3}$$

$$k \cdot \partial\phi/\partial\{n\}|_{\Gamma_2} = -q \text{ (second type)} \tag{4}$$

in which $\{n\} = \{l_x, l_y, l_z\}^T$ are direction cosines of the external normal to the boundary, ϕ_0 (L) and q ($\mathrm{L\,T^{-1}}$) are specified hydraulic potential at the first type boundary Γ_1, and the flow rate through the second type boundary Γ_2, respectively.

2.2.2. Discretization of the FE model

For a refined and elegant simulation using FEM, the efficient discretization scheme of the generated concrete sample is demanded. Since the 3D RAS is a heterogeneous random model, the geometry of the mesostructure is usually complicated. In order to improve the mesh quality and solution efficiency, the two main phases of the model, aggregates and mortar, are meshed together with tetrahedral solid elements. In FE analysis, both the aggregates