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A meso-scale model for analyzing the chloride diffusion of concrete subjected to external stress

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HIGHLIGHTS

- A meso-scale model is prosed to predict the effect of stress on diffusivity.
- The N-layered sphere model is used for predicting diffusion coefficient.
- Porosity is treated as the main parameter influencing the diffusivity in concrete.
- The quantitative relation between volumetric stress and diffusivity is given.

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ABSTRACT

This paper proposes a theoretical model to investigate the influence of low stress on the chloride penetration in concrete by modeling concrete at the meso-scale. At the meso-scale, concrete is modeled as a 3-phase composite material composed of mortar, interfacial transition zone (ITZ) and coarse aggregate. Each phase is further simplified as 2-phase composite material composed of matrix phase (zero porosity) and pore phase (the sum of various scale pores). Chloride permeability of concrete at low deformation is closely related to the porosity of concrete. Low stress changes the porosity of concrete thus influencing the chloride ion diffusion coefficient. Based on the theory of elasticity, an analytical model is developed, and a quantitative relationship is proposed between the external equivalent stress and the diffusion coefficient of the chloride ion as well as current-state porosity of mortar and the ITZ. The good agreement between the proposed model and the available test data illustrates that the proposed model is reliable and accurate. However, as the initial assumption was for elastic state, the model is valid for elastic low stress, or the accuracy of model reduces using plastic high stress state.

1. Introduction

Reinforced concrete structures in chloride salt environments generally suffer from the corrosion of reinforcement steel. Corrosion of steel can reduce the cross-sectional area of rebar (reinforcement steel) and diminish its bonding capability with concrete, which can jeopardize the longevity of the structures [1]. To date, many researchers have focused on the durability problem of concrete caused by chloride ion penetration.

Efforts have been made to explore the chloride diffusivity in concrete from a macro-scale perspective in which concrete is considered as a homogeneous material [2–5]. However, by recognizing the heterogeneity of concrete as an important factor for chloride penetration, scholars have increasingly focused on the chloride penetration of concrete from a meso-scale perspective. For instance, a meso-scale numerical model was developed to investigate the chloride diffusivity in concrete [6]. The study [6] found that both the distribution and the shape of aggregate particles have a negligible influence on the chloride diffusivity in concrete. Branko[7] proposed a three-dimensional lattice model to simulate chloride transport in saturated sound and cracked concrete. In their study, means of computationally determining transport properties of individual phases in heterogeneous concrete (aggregate, mortar, and interface) are presented and discussed.

However, studies are often performed with no consideration of the chloride penetration of concrete subjected to external stress. The diffusivity of concrete at a stress state may be significantly different from that at a stress-free state [8–10]. The porosity of mortar, interfacial transition zone (ITZ) and coarse aggregate may change under stress, and even formation of cracks within concrete

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causes changes in the permeability of concrete. Therefore, research on the chloride penetration in concrete subjected to a stress state is essential.

Most of the existing literature focused on the macro empirical model of chloride diffusion coefficient varied with stress level based on the experimental results, for instance, Wang [9] proposed a macro empirical model to predict the chloride diffusion process under different loading conditions. Konin et al. [11] carried out an experiment to investigate the chloride diffusivity of concrete subjected to tensile load. The experimental data showed that the chloride diffusion coefficient increases with the increase in the tension stress and the higher the concrete strength grade, the smaller the chloride ion concentration of penetration. To date, few scholars have investigated the chloride penetration of concrete subjected to external stress from the meso-scale and micro-scale perspectives. Bernard [12] presented a 3D numerical model in order to investigate the influence of ITZ on the compressive strength and on the effective diffusion coefficient when concrete was under uniaxial compressive stress. Du [8] and Jin [10] derived an analytical solution among the diffusion coefficient of the chloride ion, the current porosity of concrete and the external volumetric strain, however, the selection of parameters is not convenient in the Du [8] and Jin [10] models, the practical engineering tends to be more likely to get external stress, rather than strain. To sum up, there exists very limited documentation on the micro-/meso-scopic model based on the theoretical analysis of the effect of external mechanical stress on chloride diffusivity in concrete. The quantitative relationships based on a micro-scale mechanism among the diffusion coefficient of the chloride ion, the current porosity of concrete and the external equivalent stress have not been fully understood. The objective of this paper is to further clarify those quantitative relationships.

In this study, it is assumed that under the external loadings the concrete is in the elastic stage, namely, before new cracks occur. By modeling concrete at the meso-scale, concrete is simplified as a three-phase sphere composed of mortar, ITZ and coarse aggregate. Based on the theory of elasticity, an analytical model is developed. A quantitative relationship is proposed between the current-state porosity of each phase and the diffusion coefficient of the chloride ion, as well as the external equivalent stress of each phase is evaluated. With the help of finite element method analysis, the model also reveals the meso-scale phenomenon of chloride ion penetration of concrete subjected to external stress.

2. Three-phase elasticity model for determining the effective diffusion coefficient

2.1. Mesoscopic model structure of concrete

In a mesoscopic finite element analysis of concrete member, one needs to first establish a reasonable concrete mesoscopic numerical model. At the meso-scale, concrete is simplified as a composite material of three phases, namely, mortar, ITZ and coarse aggregate. The key to build a mesoscopic numerical model of concrete is appropriately determine the 3-phase composition as shown in Fig. 1.

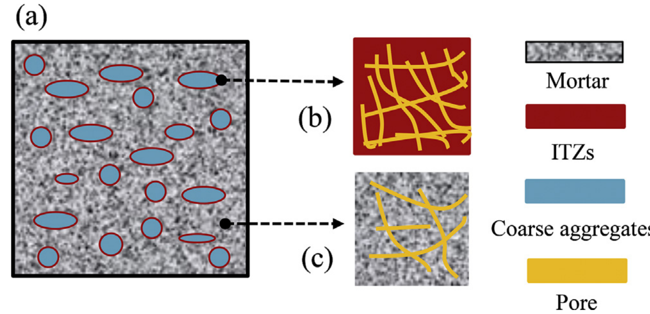

Fig. 1. Meso-scale physical analysis model of concrete.

2.1.1. Mortar

Mortar is a kind of a typical porous composite material that involved cement, water and fine aggregate. The mechanical properties were considered it as a homogeneous elastomer.

2.1.2. Coarse aggregate

Coarse aggregate is a major component of concrete that occupies approximately half of the volume of concrete [6,13,14]. A key concern in the mesoscopic modeling of concrete is how to model coarse aggregate particles by considering the shape of coarse aggregate particle, volume fraction of coarse aggregate, and the relative positions of different particles within the concrete mass. Wang [15] and Schutter [16] showed that Fuller's gradation curve makes concrete better meet the demand of strength and compactness. Du [6] and Abyaneh [17] revealed that the effect of coarse aggregate shape on the chloride ion diffusion is negligible. Therefore, for simplicity, coarse aggregate particles were modeled as circular solid particles surrounded by mortar, and were simulated for the relative position by the Monte Carlo simulation method.

2.1.3. Interfacial transition zone (ITZ)

Concrete is a multiphase composite material in which aggregate particles are embedded in mortar. Farran [18] observed that the porosity near the surface of aggregate particles in concrete is greater than the far field mortar and proposed that "Interfacial transition zone (ITZ)" exists in concrete as a zone that is relatively loose, has a low density, and is prone to cracking under external loading. From the formation viewpoint, ITZ is mainly caused by the wall-effect. ITZ as the weakest link in concrete and has a thickness of about 30—100 μm around aggregate particles [19,20]. The porosity of ITZ decreases with the increase of distance from the aggregate surface [21]. In the numerical model, however, the ITZ was considered as a uniform region. Although ITZ is relatively small, its effect on the performance of concrete can be substantial. For instance, when the volume fraction of ITZ increased by 50%, the elastic modulus of concrete was reduced by 40% [22]. Ollivier [23] believed that the characteristics of concrete largely depends on the local properties of ITZ. Nilsen [24] founded that the two-phase models of concrete, which do not consider ITZ, cannot predict the concrete properties very well.

Based on literature [9] of the following validation model, the "Series A" was selected. Series A was based on OPC, with a coarse aggregate content of 1116 kg/m^3 and a water/cement ratio of 0.5. According to the test, the volume fraction of coarse aggregate $f_{agg} = 41\%$ of concrete was derived. The mesoscopic structure modeling of concrete was performed as shown in Fig. 2.

2.2. The volumetric stress of the meso-scale components

Multi-phase spherical models have been widely utilized to calculate the apparent diffusion coefficient of concrete [8,25,26]. Based on the theory of the multi-phase spherical model, concrete was modeled as a 3-phase spherical system comprising of mortar, ITZ and coarse aggregate (Fig. 3). The elastic moduli of mortar, ITZ and coarse aggregate are denoted, respectively, as E_c, E_b and E_a, and their Poisson's ratio are denoted, respectively, as υ_c, υ_b and υ_a.

Fig. 4(b) presents the deformation behavior of concrete when subjected to the prescribed equivalent stress q_c. In Fig. 4, the