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Ionic transport features in concrete composites containing various shaped aggregates: a numerical study

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ABSTRACT

The service life of concrete-based infrastructure and buildings is seriously shortened due to the chloride-induced durability problems. In order to clarify the transport mechanism associated with the response of inclusion structures, this paper presents a numerical study on the influence caused by morphology and heterogeneity of individual phases, in which the concrete is treated as a three-phase composite including mortar, aggregates and interfacial transition zone (ITZ). A series of meso-scale numerical models with different shapes and volume fractions of aggregates are developed for examining the effects of aggregates on ionic migration. Unlike in most of the existing published research work in this area, a multi-component ionic transport theory which takes ionic interactions into consideration has been utilised in this study. By coupling mass conservation and Poisson's equations, the time-spatial concentration distribution results for individual ionic species are obtained. Other important factors such as the externally applied electric field, concrete heterogeneity, ionic binding and ITZ are also considered and examined in this study. Through this relatively thorough numerical analysis, some important features about the effect of aggregate shape based on multi-species modelling, which have previously not been properly investigated, are highlighted.

1. Introduction

Concrete is the most widely used man-made material in modern construction industry. However, the service life of concrete-based infrastructure and buildings has been seriously shortened due to the durability problems, especially the corrosion of reinforcement caused by the penetration of chloride ions. Once the chloride concentration around the reinforcing steel reaches a threshold value, depassivation of the reinforcement will occur [1,2]. To this end, it is important to clarify the transport mechanism associated with changes in ionic concentration in concrete, and how individual phases in concrete composites behave during chlorides penetration.

During the last few decades, a number of studies have been produced around the theme of assessment of ionic transport in concrete by using traditional methods, including analytical models [3–10] and experimental techniques [11–23]. Concrete is a composite material consisting of meso- and micro-structural organisations, which has a complicated heterogeneous nature. Unfortunately, most of the previous analytical studies are only capable of tackling one dimensional transport problems in a single-phase medium and are generally suitable for cement or mortar matrices, but not for concrete. Experimental studies have the advantage of providing credible and valuable data on transport properties of concrete; however, they are weak in clarifying the individual effects of different factors, as well as usually being time-consuming and expensive.

It seems that none of these earlier experimental or analytical methods is suitable for evaluating the influence of individual components on chloride transport in concrete. To deal with this, from the mechanics point of view, if the properties of each individual material involved in the concrete are known then the properties of the concrete composite should be predictable. For this concern, advanced numerical concrete models, which are originally developed for structural stress analysis [24,25], have recently been uti-

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lized to investigate the ionic transport properties of concrete, treating it as a multi-phase composite material [26–42]. By using these multi-phase computational models, it can be easy to clarify and quantify the influence of the different component parts of concrete, i.e. coarse/fine aggregate inclusion, mortar/cement and interfacial transition zones (ITZs), which could not be achieved with one dimensional (1-D) analytical models. However, most of the existing modelling work assumes that the shape of an aggregate particle is circular or spherical. This rough simplification may cause simulation results to be inaccurate. More recently, meso-structures of concrete with several aggregate shapes have been established to explore the effect of aggregate shape on the durability properties of concrete. As a typical example, Larrard et al. [44] numerically generated 3-D, 2-phase samples with and without steel bars to study the effects of the aggregate shape on drying and atmospheric carbonation. It was found that, regarding macroscopic indicators, the influence of the coarse aggregate shapes appears negligible when compared to the effect of their volume fractions. Li et al. [45] established 3-D meso-scale models to investigate the effective permeability during steady state flow, and claimed that the tortuosity effect is more pronounced when different aggregate shapes are employed. Abyaneh et al. [46] numerically explored the effect of aggregate size, shape and volume fraction on the capillary absorption. They solved the non-linear, non-steady state Fick's equation in a 3-D mesoscale model and found the shape of aggregate particles may have a significant effect on the water penetration profile and sorptivity. Using chloride diffusivity as a durability indicator, Zheng et al. [39] applied a 2-D, 3-phase model using lattice method to investigate the effect of aggregate shape on chloride diffusion through concrete, in which the aggregate particles are assumed to be elliptical. They concluded that the chloride diffusivity in concrete decreases with an increase in the aspect ratio of elliptical aggregate particles. Abyaneh et al. [47] conducted a series of numerical simulations with a 3-D finite difference model to study the effect of the shape of various spheroidal aggregates (i.e. spherical, tri-axial ellipsoidal, prolate spheroidal and oblate spheroidal). The results showed that the diffusivity decreased significantly when spherical aggregate particles were replaced by ellipsoidal aggregate particles, particularly for higher aggregate fractions and aspect ratios.

Most of transport models described above focus on the diffusion mechanism and employ Fick's law to describe the steady-state chloride diffusion in concrete with spheroidal aggregates. The ionic transport behaviour in saturated electrolyte solution is classified into both diffusion and migration, particularly for cases where an externally applied electric field is involved, such as in the rapid chloride permeability/migration test (RCPT/RCM) [21–23], and the electrochemical chloride removal (ECR) treatment [48]. The former is one of the most widely used test methods in durability testing; whereas the latter has recently become a popular rehabilitation method due to both its cost and efficiency. It is clearly essential for the numerical models to extend the ionic diffusion to a more complicated migration dominated process. In recent years, great efforts have been made on this issue [49–67]. However, the presence of an external electric field, and coupling between different species leads the transport equations to a highly nonlinear form. In order to achieve convergent solutions, most existing numerical simulations regarding migration only adopt a 1-D model or 2-D model, but incorporate a number of simplifications (e.g. circular aggregates).

The above literature review shows that the influence of inner structures morphology, i.e., various shaped aggregates on ionic transport in a multiple ionic electro-migration process within mortar or concrete has not been investigated in the existing models. In this paper, a numerical study is presented to simulate the chloride migration process by treating the concrete as a three-phase composite including mortar, ITZs and aggregates with various shapes and volume fractions. A series of meso-scale models are developed for a theoretical investigation. The previous studies on the effect of aggregate shape [39,47] did not discuss or show the details of chloride transport in concrete, such as the time-dependent concentration distribution and penetration depth (which are the key information for predicting the depassivation process or chloride diffusivity), and they modelled concrete with only spheroidal shaped inclusions. The study presented in this paper examines both spheroidal and polygonal aggregates, and also provides time-spatial distribution results for the four ionic species involved (K^+, Na^+, Cl^-, OH^-) by solving coupled mass conservation and Poisson's equations. Other important factors such as the externally applied electric field, concrete heterogeneity, ionic binding and the ITZs are also considered and examined in this study. Through this thorough numerical analysis based on multi-phase and multi-species modelling, some important features about the effect of aggregate shape, which have not previously been properly investigated, are highlighted.

2. Theoretical background

In order to discuss the ionic transport features in heterogeneous concrete subjected to an external electric field, more attention should be devoted to the definitions of driving forces, ionic binding, time-dependent concentration and electrical potential per unit of medium.

Fick's law is not adequate to describe the ionic transport other than the diffusion process. When a transport process includes various driving forces such as concentration gradient, electric field, pressure flow and chemical activity, the flux of ionic species can be presented by the extended Nernst-Planck equation as follows,

$$\mathbf{J}_k = -D_k \nabla C_k - \frac{z_k F}{RT} D_k C_k \nabla \Phi + C_k u_k - \frac{C_k}{\gamma_k} \nabla \gamma_k \tag{1}$$

where $\mathbf{J}_k$ and C_k are the flux and the concentration of the kth species, respectively, D_k is the diffusion coefficient, u_k is the advective velocity, γ_k is the chemical activity coefficient, z_k is the charge number, $F = 9.648 \times 10^4\ \mathrm{C mol^{-1}}$ is the Faraday constant, $R = 8.314\ \mathrm{J\ mol^{-1}\ K^{-1}}$ is the ideal gas constant, $T = 298$ K is the absolute temperature, and Φ is the electrostatic potential. For the RCM test, as the pore solution is fully saturated with diluted solution and there are no pressure differences, the terms of convection and chemical activity can be ignored. Hence, the extended Nernst-Planck equation can be simplified to a diffusion-migration form, as follows:

$$\mathbf{J}_k = -D_k \nabla C_k - \frac{z_k F}{RT} D_k C_k \nabla \Phi \tag{2}$$

To quantitatively describe the time-spatial distribution of ionic concentrations, each ionic species involved in the electrolyte solution is also subjected to the mass conservation equations as described in Eq. (3),

$$\frac{\partial C_k}{\partial t} = -\nabla \cdot \mathbf{J}_k \tag{3}$$

where t is time. As the effect of the aggregate is involved in this study, the concrete considered here is modelled as a composite structure consisting of aggregate-, cement paste- and ITZ-phases at mesoscopic level. The cement paste phase and ITZ phase are treated as two different porous materials; different microstructure properties are applied in the numerical simulation to show their different transport properties. Thus the governing equations for ionic transport in this study should be rewritten and taken influences of the microstructure properties of the porous materials into account. In this study, porosity and tortuosity of the pore structure

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