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A three-phase, multi-component ionic transport model for simulation of chloride penetration in concrete

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ABSTRACT

Chloride-induced corrosion of reinforcing steel in concrete is a serious problem in the durability of structures. In order to predict how chlorides penetrate in concrete, unlike most existing models which consider the penetration of only a single species or in a single phase medium, this paper presents a numerical model considering the transport of multiple species in a multi-phase medium. The 2-D, 3-phase, multi-component ionic transport model proposed in the paper also considers ionic binding and the model is used to simulate the rapid chloride migration (RCM) test of concrete. The effects of aggregates, ITZs and ionic binding on chloride penetration in concrete are examined and discussed. The obtained result is also validated against experimental data obtained in an accelerated chloride migration test.

1. Introduction

Chloride-induced corrosion of reinforcing steel in concrete is a worldwide problem. It affects a large number of reinforced concrete structures, particularly those used in offshore or exposed in marine environment. In order to prevent reinforcing steel from corrosion one has to control the penetration of chlorides in concrete. By doing so, one has to know the mechanism about how chlorides penetrate in concrete and how individual components in concrete respond while chlorides enter the concrete.

Concrete is a composite material composed of aggregates embedded in a hard matrix of the cement paste that fills the space among the aggregates and glues them together. The cement particles in fresh concrete, which are suspended in the mix water, cannot pack together as efficiently when they are in the close vicinity of a much larger solid object, such an aggregate particle. This is due to the effect of shear stresses exerted on the cement paste by the aggregate particles during mixing, which tend to cause the water to separate from the cement particles. This results in a narrow region around the aggregate particles with fewer cement particles, and thus more water. This narrow region is usually called the interfacial transition zone (ITZ) [1–3].

ITZ has a higher water-to-cement ratio and thus a larger porosity, than the bulk cement paste. Images of SEM have shown that ITZ is not uniform, but varies with the distance from the aggregate particle [4,5]. The average thickness of ITZs found in a normal concrete is 20–40 μm, although it tends to be larger around larger aggregate particles. The ITZ has important effects on the mechanical properties and durability of concrete, because it tends to act as the "weak link in the chain" when compared with the bulk cement paste and the aggregate particles.

Extensive research has been carried out since early of 1980s to investigate how chlorides penetrate in concrete. The work involves the use of analytical, experimental, and numerical methods. The corresponding transport models so far developed can be categorised into four groups, as illustrated in Fig. 1. The first group is the transport model considering the penetration of a single species (i.e. chloride ions) in a single phase medium (i.e. idealised dilute solution) [6–11]. The second group is the transport model considering the transport of multiple species (such as chloride, hydroxyl,

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sodium and potassium ions) also in a single phase medium [12–21]. The third group is the transport model considering the penetration of a single species in a medium of multiple phases with different transport properties [22–37]. The forth group is the transport model considering the transport of multiple species also in a medium of multiple phases [38]. The models used in the third and fourth groups are also called the multi-phase model.

The main purpose of developing multi-phase transport models is to numerically investigate the effect of individual components of concrete such as aggregates and ITZs on the transport of chlorides, which cannot be fulfilled by using the 1-D model. For example, Zeng developed a 2-D, 2-phase FEA model to simulate the chloride diffusion in a heterogeneous concrete composed of aggregates and cement paste matrix, which have distinct chloride diffusivities [39]. His result showed that the chloride diffusion in the heterogeneous concrete lags behind the equivalent homogeneous concrete chloride diffusion predicted using an effective diffusion coefficient. Zheng and Zhou proposed a 3-phase spherical model to represent the heterogeneous nature of concrete and derived an analytical expression for chloride diffusion in concrete [40]. Later, Zheng et al. further investigated the influence of ITZs on the steady-state chloride diffusion in mortar and concrete materials using numerical simulations [41]. Recently, Zheng et al. developed a 2-D, 3-phase lattice model and investigated the shape effect of aggregates on chloride diffusion in concrete [42]. Li et al. developed 2-phase FEA models in both 2-D and 3-D to predict the effect of aggregates on the effective diffusion coefficient of chlorides [43]. Their result showed that the 2-D model produced a lower chloride diffusivity of concrete than the 3-D model does. The former is close to the lower bound of the effective diffusion coefficient of chlorides in concrete, whereas the latter agrees with that predicted by using Maxwell's equation. More recently, Abyaneh et al. developed a 3-D, 3-phase FEA model to investigate the effects of aggregates including the aspect-ratio and orientation of ellipse shape aggregates and ITZs on the diffusion coefficient of chlorides in concrete [44]. The effect of electrical double layer on ionic transport in cement-based materials was also investigated recently [45,46].

Note that most multi-phase numerical models mentioned above [39–44] also consider the penetration of only chloride ions. The interaction between different ionic species is not taken into account in these models. Existing studies have shown that ionic interactions have an important effect on the transport of chlorides in concrete, particularly when there is an external electric field involved [17–21]. Typical examples for such cases include the rapid chloride migration (RCM) tests and electrochemical chloride removal. In the previous 2-D, 2-phase FEA model [38] we considered the interaction between different ionic species and examined the effect of aggregates on the transport of various ionic species in concrete. However the model did not include ITZs and ionic binding. In this paper the previous 2-D, 2-phase FEA model [38] is further expanded to include ITZs and to take into account the ionic binding. The present 2-D, 3-phase, multi-component ionic transport model is used to simulate the RCM test of concrete, from which the effects of aggregates, ITZs and ionic binding on chloride penetration in concrete are discussed.

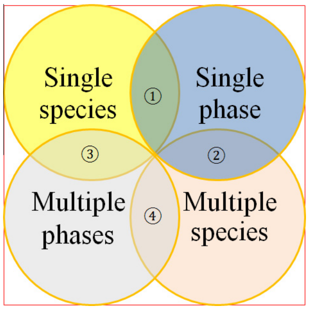

Fig. 1. Categories of ionic transport models in concrete. (1) Single phase and single species transport model, (2) single phase and multi-species transport model, (3) multi-phase and single species transport model, and (4) multi-phase and multi-species transport model.

Ideally, the multi-phase modelling of ionic transport in concrete should use a 3D geometric model, for example [44,47,48]. However, at present the 3D model can be applied only to the problems where the model has a single ionic species [44,47] or multiple ionic species but they are controlled by the electro-neutrality condition [48,49]. The reason for this is because in either case the migration speed is independent of ionic concentration, for which case the governing equations are linear and their solution can be achieved without numerical difficulty. However, the use of electro-neutrality condition leads to a decoupling of ionic transport between different ionic species, which is principally incorrect [20,50]. Therefore, one should use the Poisson equation, instead of the electro-neutrality condition [20,21,38]. The use of Poisson equation in the ionic transport model makes the transport equations not only highly nonlinear but also the coupling between different ionic species. As a consequence of this, the migration speed of individual ionic species may vary greatly with time and position. This makes very difficult to achieve convergent solutions unless the element sizes in the finite element mesh are extremely small [38,47]. This problem even gets worse when the ITZs are involved in the model. This is why most multiphase models, available today, use the 2-D rather than 3-D geometry. Note that although the variation of tortuosity with volume fraction in a 2-D geometry is not exactly the same as that in a 3-D geometry, the difference is not very significant [47,50]. Thus, the 2-D simulation can provide a good approximation, while the 3-D simulation results are not available.

2. Ionic transport in multi-component electrolyte solutions

The pore solution in concrete involves many ionic species including hydroxyl, sulphate, sodium, potassium, calcium, etc., among which the hydroxyl has the highest concentration, followed by the potassium and sodium. The transport of ions in a saturated concrete is mainly by two driving forces, known as the diffusion and migration. The former is due to the concentration gradient of the species itself; the latter is due to the electrostatic potential generated by an externally applied electric field and/or the internal charge imbalance between different species in the solution. In the presence of external electric field, positively charged ions will move towards cathode, whereas negatively charged ions will move towards anode. The opposite-direction movement between cations and anions will generate significant internal charge imbalance between cations and anions within the solution. This charge imbalance creates an electrostatic potential which can affect the transport of all ionic species in the solution. In the absence of external electric field, different ionic species having different diffusion coefficients travel in different speeds. This also generates charge imbalance between species and creates an electrostatic potential, which affects the transport of all ionic species in the solution. The exact effect of charge imbalance on the transport of ions in concrete is dependent on the external electric field applied and the difference of diffusion coefficients between ionic species. In general, the effect of charge imbalance on the ionic transport increases with the external electric field and the difference of diffusion coefficients between ionic species. Mathematically, the flux of an ionic species in a multi-component electrolyte solution can be expressed in terms of Nernst–Planck equation as follows,

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