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Modelling of chloride ingress into concrete from a saline environment

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Abstract

A mathematical model previously developed for the simulation of electrochemical chloride removal (ECR) process is utilised to predict the ionic mass transport associated with chloride ingress into concrete or hydrated cement paste from a saline environment by incorporating the convection of pore solution. Compared to the existing models, the present model has advantages in the aspect of numerical calculations as it avoids the difficulty of solving the Poisson equation about electrostatic potential. The significant effects of ionic interaction and the convection of pore solution on the chloride ingress are examined. Simulation results are compared with those obtained from the models using Fick's second law. The comparison shows that the present model is more detailed and accurate. It can be applied to various different cases with unified ionic diffusivities.

Keywords: Chloride ingress; Diffusion; Concrete; Mathematical model; Finite element method

1. Introduction

Corrosion of reinforcing steel in concrete due to chloride ingress is one of the main causes of the deterioration of reinforced concrete structures, particularly in marine environments. It is therefore desirable to develop methods, which can be used to simulate the chloride ingress process and predict the chloride concentration profiles accurately to help to assess the service condition for reinforced concrete structures. In the past decades, both physical and computer models were developed to investigate the process of chloride ingress. At the early stage of the modelling, Fick's second law was widely adopted, in which the concentration gradient was assumed as the only driving force of the transport of chloride ions in concrete [1–6]. Recently, more comprehensive models have been proposed to take account of individual factors related to the chloride transport in concrete systems. These factors include the diffusion of different types of ions in pore solution, the unsaturated moisture flow in pore structure and the mass exchange between ions in pore solution and in solid hydration products in concrete such as the binding and leaching of chloride, hydroxide and calcium ions [7–13]. Parallel to the development of the above models, similar models were developed for the simulation of electrochemical chloride removal (ECR) by Yu and Page [14], Li and Page [15–17] and lately by Wang et al. [18]. Different from those proposed by Samson et al. [8], Marchand [9] and Jahannesson [10,11], however, these ECR models did not employ Poisson equation on the determination of electrostatic potential. Numerically, there is a difficulty in solving the electrostatic potential if the Poisson equation is employed because it involves a very large number, F/ε, with the order of 10^{16}.

In this paper, we develop our previous ECR model by incorporating the effect of the bulk solution flow in pore structure. The model, then, can be applied to predict the chloride ingress into concrete from a saline environment by simply cancelling the activity of the external electrical

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field which is in action in ECR cases. Unsaturated flow theory is utilised to determine the convection of the pore solution. The governing equations in the model are solved using the finite element method (FEM). As an application, the model was used to simulate a published chloride ingress experiment. The effects of the interaction between the different ionic species and the convection of pore solution on the chloride ingress are examined. The modelling results are compared with those obtained from the traditional models using the second Fick's law.

2. Mathematical model of ionic transport in porous media

In a previously proposed ECR model, when the concrete is regarded as saturated, ignoring the flow of bulk solution, the transport of ionic species in it can be described using the following [15–18]:

$$\tau^2 \frac{\partial}{\partial t}(C_i + S_i) = z_i \frac{F}{RT} \nabla(D_i C_i \nabla\phi) + \nabla(D_i \nabla C_i), \tag{1}$$

$$\frac{F}{RT}\nabla\phi = -\frac{\frac{\tau \boldsymbol{I}}{\varepsilon^{2/3}F} + \sum_i^n z_i D_i \nabla C_i}{\sum_i^n z_i^2 D_i C_i}, \tag{2}$$

where C_i is the concentration of species i in solution, S_i the concentration of bound ions of species i, z_i the charge number of species i, F the Faraday's constant, R the gas constant, D_i the diffusion coefficient in solution, ϕ the electrostatic potential, $\boldsymbol{I}$ the current density caused by an externally applied electrical field, n the total number of the species in solution, τ the tortuosity of pore structure, ε the volume fraction of porosity.

The two terms on the right-hand side of Eq. (1) represent the two mechanisms of the ionic transfer. They are the migration of ions due to electrostatic potential gradient and the diffusion of ions due to ionic concentration gradient, respectively.

If the pore structure is not saturated initially, when it is in contact with a body of water we need to consider the influence of the flowing of the bulk pore solution due to water infusion [8,9]. As a result, Eqs. (1) and (2) need to be modified and the modified equations can be expressed as

$$\tau^2 \frac{\partial}{\partial t}(C_i\theta + S_i\theta) = z_i \nabla\left[D_i\left(\frac{F}{RT}\nabla\phi\right)C_i\theta\right] + \nabla(D_i\nabla(C_i\theta)) - \tau\nabla(C_i\theta\mathbf{v}), \tag{3}$$

$$\frac{F}{RT}\nabla\phi = -\frac{\frac{\tau \boldsymbol{I}}{F\varepsilon^{2/3}} + \sum_i^n z_i D_i \nabla(C_i\theta)}{\sum_i^n z_i^2 D_i C_i\theta}, \tag{4}$$

where $\mathbf{v}$ is the velocity of bulk solution, θ the saturation of the pore structure.

The concentration of bound ions is normally expressed as a function of the concentration of free ions and water saturation, i.e., $S_i = f(C_i, \theta)$. The water saturation is expressed as the volume fraction saturated at time t. A detailed discussion about saturation will be given in a later section. In the case of chloride ingress into concrete the current density, $\boldsymbol{I}$, is generally taken as zero because there is no externally applied electrical field.

3. Finite element analysis

Eqs. (3) and (4) are the transient non-linear convection–diffusion equations with variable coefficients, which can be solved numerically by using FEM [15,19]. For one-dimensional problems, one can take $C_i\theta$ together as an integral independent variable and use the linear interpolation function to construct the distribution of this variable as follows

$$C_i(x,t)\theta(x,t) = \sum_{j=1}^{2} N_j(x)(C_i\theta)^j = \boldsymbol{N}\{(C_i\theta)^j\}, \tag{5}$$

where $\boldsymbol{N} = [N_1, N_2]$: shape function matrix for a two-node element, j is the nodal number of an element, $\{(C_i\theta)^j\} = [(C_i\theta)^1, (C_i\theta)^2]^{\mathrm{T}}$: nodal vector.

The rate of the generation of bound ions can be expressed as a function of the rate of free ions as follows

$$\frac{\partial(S_i\theta)}{\partial t} = \frac{\partial(S_i\theta)}{\partial(C_i\theta)}\frac{\partial(C_i\theta)}{\partial t} = \lambda(C_i,\theta)\frac{\partial(C_i\theta)}{\partial t}, \tag{6}$$

where λ is the relation-function between the concentration rates of free and bound ions.

Before solving Eqs. (3) and (4) to obtain the ionic concentration, we must know the saturation of the pore structure, θ, and the velocity of bulk solution, $\mathbf{v}$, which are discussed in the following section.

4. The theory of water transport in porous materials

For ideal, dilute solution, the transport of ionic solution can be approximately treated as the transport of water. If neglecting the osmotic effect of ionic concentration on the transport of water, the ionic solution ingress into unsaturated porous media can be simplified as water ingress. It is known that the cause for water flowing through a porous medium could be the pressure gradient and/or capillary forces. Mathematically, the former can be described by employing Darcy's Law [20,21], while the latter can be described by means of the unsaturated flow theory [22]. According to the unsaturated flow theory, the water flow velocity can be expressed as follows [23]

$$\boldsymbol{q} = -D_{\mathrm{w}}(\theta)\nabla\theta, \tag{7}$$