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Modeling of chloride diffusivity coupled with non-linear binding capacity in sound and cracked concrete

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ABSTRACT

The objective of this research is to establish a model that can predict chloride transport phenomena in sound and cracked concrete. The chloride diffusivity is formulated based on computed micro-pore structure, which considers tortuosity and constrictivity of porous network as reduction factors in terms of complex micro-pore structure and electric interaction of chloride ions and pore wall. In the real environment, concrete structures are not always crack-free, therefore chloride transport in cracked concrete is also simulated by section large void spaces in a control volume to represent the crack and by proposing a model of chloride diffusivity through the cracked region The proposed models are implemented into a finite-element computational program DuCOM, which simulates the early-age development process of cementitious materials. The calculated concentration profiles of total chloride ions are verified through a comparison with experiments results.

1. Introduction

For structures exposed to sea water and/or deicing salt, chloride penetration is a common cause of deterioration of reinforced concrete. In order to predict the service life of such structures, it is necessary to quantify the chloride transport process in cementitious materials. It is well known that binding capacity and chloride diffusivity have a significant effect on the chloride diffusion process. In this study, the chloride binding model describing the equilibrium between chloride ions and bound chlorides is modeled as a non-linear function based on Langmuir's equation. The non-linear binding model gives an inflection point in computed chloride distributions, which is not observed in real measurement. This is the fact that a couple of researchers have already found in the past literatures [1]. In this study, through several sensitivity analyses, the authors show that the non-linear binding model considering the constrictivity factor in diffusion model gives reasonable agreement with the measured profile. The constrictivity factor not only considers the effect of ion and pore wall interaction but also considers the interaction of diffusing ions with bound chloride components.

In the real environment, concrete structures are not always crack-free, and the formation of cracks increases the transport properties of concrete so that moisture along with chloride ions and oxygen easily penetrate and reach the reinforcing steel and speed up the initiation of steel corrosion in concrete. The chloride diffusion model, therefore, is extended for cracked concrete. Crack widths range from very small internal micro-cracks, to quite large cracks caused by unwanted interactions with the environment and external loading. In this research the transport of chloride ions in cracked concrete is simulated by section large void spaces in a control volume to represent the crack and by proposing a model of chloride diffusivity through the cracked region. To simulate the chloride movement in the cracked path, the chloride diffusion phenomenon is separately defined for cracked and sound concrete.

The above models are implemented into a finite-element computational program DuCOM which simulates the early-age development process of cementitious materials. The calculated concentration profiles of total chloride ions are verified through a comparison with experiment results.

2. DuCOM—a thermodynamic durability concrete model

In this research, a DuCOM model is used, which is a durability computation model developed by Concrete Laboratory at the University of Tokyo, Japan [2–4]. The originality of this model comes from the fact that the DuCOM is a composite multipurpose model, which predicts the state of the concrete from its birth to its entire life. It comprises several sub-models, which work together and are interlinked. The development of multi-scale micro-pore structures at an early-age is obtained based on the computed degree of cement hydration in the mixture. For any arbitrary initial and boundary conditions, the vapor pressure in pores, relative humidity (RH), and

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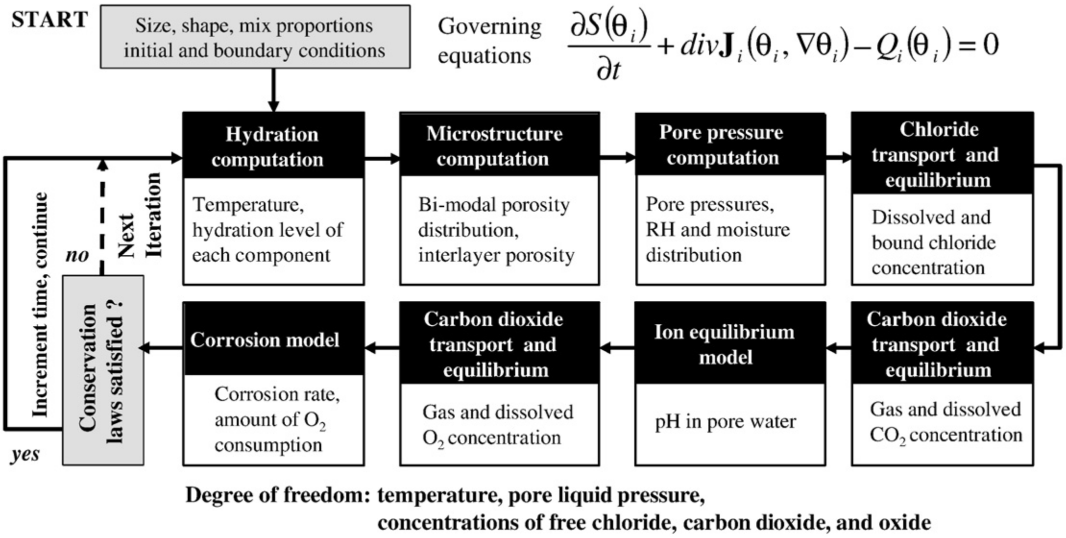

Fig. 1. Basic framework of DuCOM system [2–4].

moisture distribution are mathematically simulated according to a moisture transport model that considers both vapor and liquid phases of mass transport. The moisture distribution, RH, and micro-pore structure characteristics in turn control the Cl^-, CO_2 and O_2 diffusion and rate of various chemical reactions under arbitrary environmental conditions. In this study, the chloride transport in sound and cracked concrete is the primary focal point. An association map of the whole model is summarized as Fig. 1.

3. Governing equation for chloride ion

Chloride transport in cementitious materials under usual conditions is an advective–diffusive phenomenon. In modeling, the advective transport due to bulk movement or pore solution phase is considered, as well as ionic diffusion due to concentration gradients. Mass balance for (moveable) chloride ions can be expressed as [2–4]

$$\frac{\partial}{\partial t}(\phi S C_{\mathrm{cl}}) + \mathrm{div} J_{\mathrm{cl}} - Q_{\mathrm{cl}} = 0, \qquad (1)$$

where ϕ: porosity, S: degree of saturation of porous media, and C_{Cl}: concentration of chloride ions in pore solution, and J_{Cl}: total flux of chloride ion. The first term in Eq. (1) represents the rate of change in total amount of chloride ion per unit of time and volume, the second term is the flux of chloride ion, and the third term Q_{Cl} is a sink term. Only capillary and gel pores, which can act as transport paths for chloride ions, or locations for chemical reactions, are considered (the

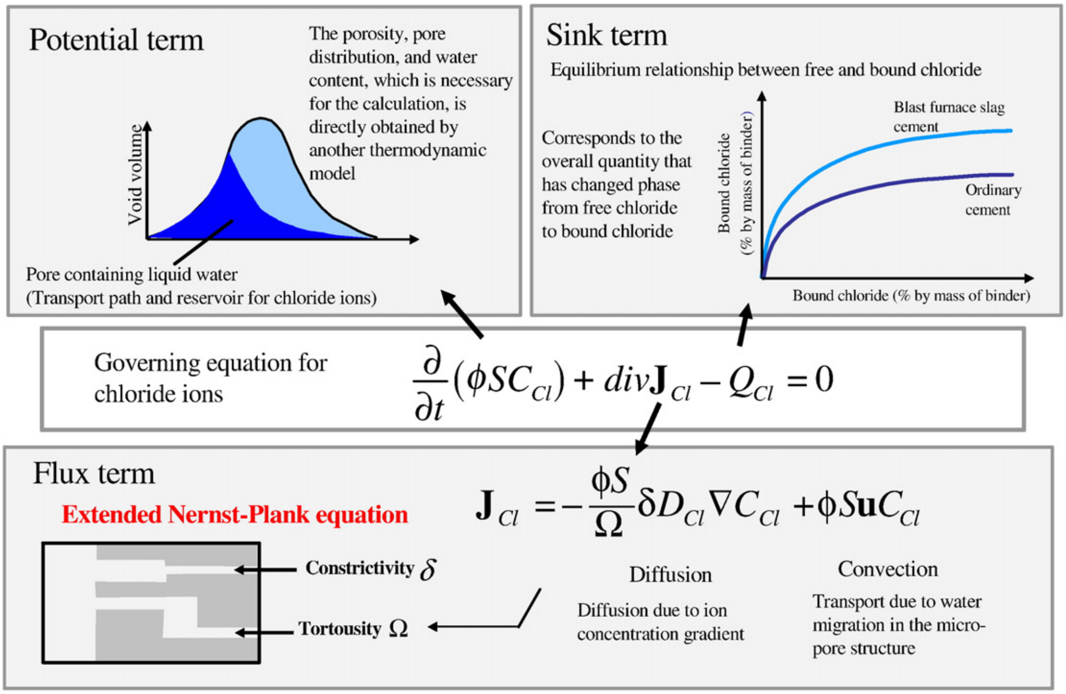

Fig. 2. Law of conservation of mass for chloride transport.