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Modelling of chloride diffusivity in concrete considering effect of aggregates

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HIGHLIGHTS

- A simple prediction model of chloride diffusivity in concrete is proposed.
- The model considers the ITZ and the aggregate shape.
- The diffusivity predicted using the model showed good agreement with test results.
- The proposed model can be effectively used to predict the diffusivity of concrete.

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ABSTRACT

In this study, a simple prediction model of chloride diffusivity in concrete is proposed. The model considers the interfacial transition zone and the aggregate shapes. An experiment was performed in which the non-steady-state diffusivity of concrete specimens with water-to-cement ratios of 0.4, 0.5, and 0.6 were measured at ages of 3, 7, 28, and 91 days. The diffusivity predicted using the model agreed well with the experimental results in this study. The proposed model is expected to be useful in realistically predicting the diffusivity of chloride in concrete.

1. Introduction

When concrete are exposed to a chloride environment, the chloride ions can penetrate the concrete, which may cause steel corrosion. The steel corrosion deteriorates the durability of the materials and the strength of the reinforced concrete structures, which may result in safety issues in the structural systems. A durability design requires accurate estimation of the initiation of the corrosion. Chloride diffusivity, which is an important parameter in predicting the initiation and propagation of corrosion in the reinforcements, varies with the concrete material properties and the environmental conditions [1,2].

A number of studies have been conducted in order to accurately estimate the chloride diffusivity of cementitious materials. Delagrave et al. [3] reported that as the aggregate content increased, the chloride diffusivity decreased. Yang and Su [4] experimentally investigated the effects of dilution, tortuosity, and the interfacial transition zone (ITZ) on the chloride diffusivity of concrete. Caré [5] conducted a migration test of mortar specimens and reported that the aggregates affected the chloride diffusivity of the specimens. In Caré's study [5], the effect of aggregates on the chloride diffusivity was taken into account by considering both the change of ITZ volume surrounded by aggregates and the change of length of pathway for chloride ion ingress in concrete. Lindvall [6] conducted tests to identify the effect of temperature on the chloride diffusivity of concrete and reported that the diffusivity increased with increasing temperature. Chalee et al. [7] confirmed that the partial replacement of ordinary Portland cement with fly-ash reduced the diffusivity of concrete. Djerbi et al. [8] studied the effects of crack width on chloride diffusion and found that the diffusivity increased with increasing crack width up to a threshold value and that it remained constant above that value. Wang et al. [9] conducted a study on changes in diffusivity as a function of density and orientation of cracks, tortuosity, and crack width. Song

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et al. [10] conducted immersion tests, in which the effect of the type of cation on the changes in the diffusivity of concrete were investigated.

Even though a variety of studies have been carried out regarding the chloride diffusivity in concrete, the aggregate effects on the diffusivity in concrete has barely been addressed. The inclusion of aggregates into the cement paste results in the formation of an ITZ around the aggregates, which is the primary pathway for chloride diffusion. Bourdette et al. [11] suggested that the ITZ is 30 μm thick, and Winslow et al. [12] reported that the porosity of the ITZ increased with increasing aggregate content. In order to predict the chloride diffusivity of cementitious materials such as mortar and concrete-containing aggregates accurately, it is important to consider the effect of the ITZ. In addition, as compared to cement pastes, aggregates are very dense, and thus the movement of chloride ions through the aggregates can be ignored [13]. However, the shapes of the aggregates need to be considered because the aggregates act as obstacles to the movement of chloride ions. Zheng et al. [14–15] studied the effect of aggregate shape on the chloride diffusivity of concrete, suggesting that the chloride diffusivity decreased with increasing aggregate aspect ratio.

In this study, a chloride diffusivity prediction model was developed that considers the effect of aggregates. The porosity of the ITZ, which was calculated using the model proposed by Pang et al. [16], was incorporated into the model. The aggregate shapes in the concrete were taken into account by using the shape function [17]. In order to validate the proposed model, an experiment was conducted in which the diffusivity of chloride in concrete with water-to-cement ratios of 0.4, 0.5, and 0.6 was measured at 3, 7, 28, and 91 days in accordance with NT Build 492 [18]. The validity of the model was confirmed by comparing the chloride diffusivity predicted using the model not only with the results of tests conducted in this study but also with experimental results reported in the literature.

2. Modeling of chloride diffusivity in cementitious materials

2.1. Cement paste

The effective diffusivity of ions is less in porous materials than in water. The normalized diffusivity of ions can be given as follows [19–22]:

$$\frac{D_e}{D_0} = \frac{\sigma_e}{\sigma_0}\phi\beta \tag{1}$$

where D_e is the effective diffusivity of ions in the materials, D_0 is the diffusivity of ions in water, D_e/D_0 is the normalized diffusivity, σ_e is the effective conductivity of ions in the materials, σ_0 is the conductivity in the saturated electrolyte, ϕ is the capillary porosity of the materials, and β is the tortuosity of the materials. The model given in Eq. (1), which was obtained by a homogenization technique based on Tanaka's approach using Maxwell's model [21], estimates the effective diffusivity of a composite material.

In this study, the chloride diffusivity of cement pastes was mathematically formulated in terms of capillary porosity. The relationship between capillary porosity and normalized diffusivity in the cement pastes was estimated based on test results reported elsewhere [23–29], as shown in Fig. 1. The value of D_0 used was 2.032×10^{-9} m^2/s at 25 °C [30].

Using the regression results shown in Fig. 1, the effective diffusivity of chloride ions in the cement pastes was modeled as follows:

$$\log\frac{D_e}{D_0} = -3.52\phi^2 + 7.52\phi - 4 \tag{2}$$

When the capillary porosity is equal to zero, D_e/D_0 is the normalized diffusivity of the materials depending on the pore structures of the hardened paste matrix. For Portland cement pastes, Oh et al. [31] suggested a D_e/D_0 value of 1.0×10^{-4}. When the capillary porosity is equal to one, D_e corresponds to the diffusivity of chloride ions in bulk water. Using Eq. (2), the chloride diffusivity can be evaluated when the capillary porosity of the cement pastes is known.

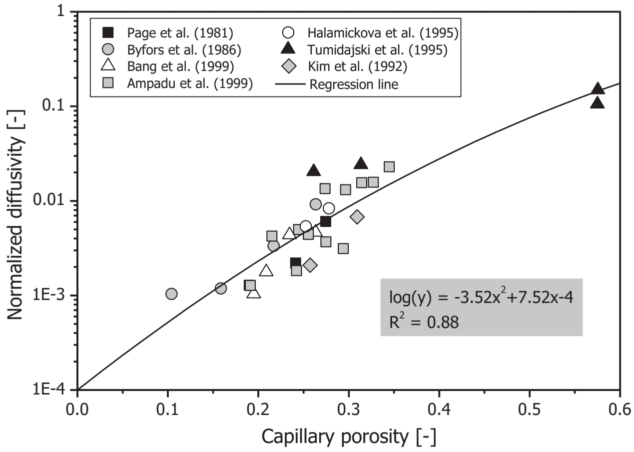

Fig. 1. Relationship between capillary porosity and normalized diffusivity in cement pastes.

Pang et al. [16] suggested the prediction model of capillary porosity in cement pastes given in Eq. (3), which includes a variety of material parameters.

$$\phi = \frac{w/c - \left[0.75k + 0.28\left(\frac{\rho_w}{\rho_c} + (w/c)^*\right)\right]\alpha}{\frac{\rho_w}{\rho_c} + w/c} \tag{3}$$

where w/c is the water-to-cement ratio, α is the degree of hydration, ρ_w is the density of water, and ρ_c is the density of the cement. k is related to amount of chemically bound water produced when the cement is completely hydrated and $(w/c)^*$ is water-to-cement ratio needed to attain complete hydration [16]. Typical values of k and $(w/c)^*$ are 0.23 and 0.38, respectively [16].

Fig. 2 shows the effective diffusivity of cement pastes as a function of the degree of hydration. The diffusivity was calculated by substituting the capillary porosity calculated using Eq. (3) into Eq. (2). As the water-to-cement ratio increased, the diffusivity of the cement pastes also rapidly increased because of the increased capillary porosity. On the other hand, the diffusivity decreased with increasing hydration of the cement pastes because of

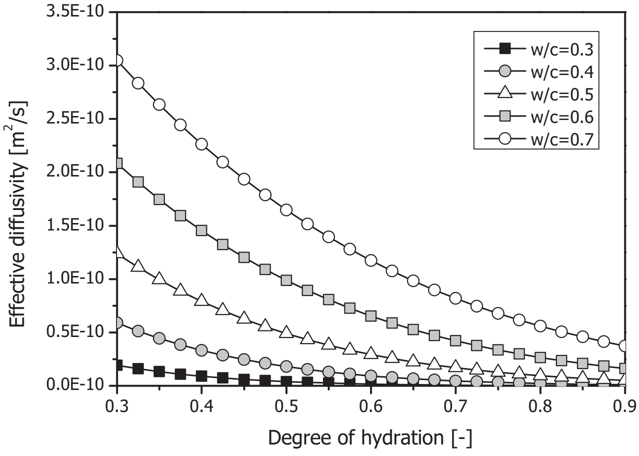

Fig. 2. Effective diffusivity of cement pastes as a function of degree of hydration.