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Experimental and cellular-automata-based analysis of chloride ion diffusion in reactive powder concrete subjected to freeze–thaw cycling

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HIGHLIGHTS

- Chloride ion diffusion coefficient calculation method has been proposed.
- Coefficient first decreased and then increased as the number of cycles increased.
- Cellular automaton-based chloride ion diffusion model was proposed.
- Model can effectively simulate and predict the chloride ion diffusion in concrete.

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ABSTRACT

Natural soaking and accelerated freeze–thaw cycling experiments were conducted using NaCl solution to study chloride ion diffusion in reactive powder concrete. The chloride ion diffusion coefficient for specimens subjected to natural soaking was calculated using Fick's second law. That for specimens subjected to freeze–thaw cycling was calculated using a newly proposed method that considers the damage resulting from freeze–thaw cycling. The coefficient first decreased and then increased as the number of cycles increased. A cellular-automata-based two-dimensional chloride ion diffusion model that considers the time dependence and impact of freeze–thaw cycling damage was established. The chloride ion diffusion and distribution in reactive powder concrete subjected to natural soaking and freeze–thaw cycling in NaCl solution were simulated using Matlab program that was based on the proposed model. The boundary condition for the cellular-automata model should be the surface chloride ion concentration instead of the chloride ion concentration of the solution. The acceleration of chloride ion diffusion due to freeze–thaw cycling damage can be well-simulated by introducing the freeze–thaw damage factor. A comparison of simulation and experimental results showed that this model can simulate and predict chloride ion diffusion in reactive powder concrete effectively.

1. Introduction

In recent years, the number of concrete structures that have suffered durability failure has progressively increased. Therefore, the durability and service life predictions for concrete structures should be considered during the structural design process. For existing structures, residual life predictions must be reliable. For this purpose, the erosion caused by harmful ions in the environment must be simulated and predicted. Freeze–thaw damage and chloride ion erosion are the primary causes of durability failure of concrete structures [1,2], and these two factors acting together accelerate damage progression.

Fick's second law is widely used for simulating and analyzing chloride ion diffusion in concrete. Yang et al. showed that the chloride ion diffusion coefficient was directly related to the aperture size [3]. Martín-Pérez et al. applied Fick's second law and took the binding effect into consideration to determine the corrected chloride ion diffusion coefficient [4]. Erdoğdu et al. used Fick's second law to analyze the chloride ion diffusion coefficients in a study using an electronic accelerating device [5]. Liang et al. applied Fick's second law and Laplace transform to study the pore chloride ion diffusion coefficient by considering the effects of an electric field and the binding effect [6]. Sun et al. predicted the service life of concrete under relatively high chloride concentrations by using Fick's second law and an irreversible first-order reaction equation by considering time dependence and the binding effect [7]. Additionally, some researchers have introduced parameters in Fick's second law to establish different models to consider the influence

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of different factors; however, these models have very complex forms.

Cellular-automata can be used to effectively solve the problems posed by complex systems without introducing the need to solve differential equations; a cellular-automaton is a discrete model of time, space, and state. Biondini et al. analyzed the durability of concrete structures in corrosive environments using cellular-automata [8]. Podroužek simulated chloride ion diffusion and predicted the service life of concrete used in a bridge structure [9]. Cao et al. modified the cellular-automata model to consider time dependence and simulated chloride ion diffusion in concrete; their simulation results showed good agreement with the experimental results [10].

Reactive powder concrete shows excellent durability [11]. It is currently being used in many engineered structures, especially bridges. It is suitable for use as the main structure or as protective material [12]. In the present study, the accelerated freeze–thaw cycling laboratory tests with 5.0 wt% NaCl solution were conducted to investigate the chloride ion distribution in reactive powder concrete under freeze–thaw cycling and the influence of freeze–thaw cycling damage on the chloride ion diffusion coefficient. The boundary conditions for a cellular-automata model with simulated natural soaking (chloride ion erosion) and freeze–thaw cycling (i.e., coupled chloride ion erosion and freeze–thaw cycling) were discussed. To consider the time dependence and freeze–thaw cycling damage, two- and one-dimensional simulations were respectively performed to simulate chloride ion diffusion conditions in reactive powder concrete subjected to natural soaking and freeze–thaw cycling. The simulation results were then compared with the experimental results. The results of this study can be used as a reference to determine chloride ion diffusion conditions and to predict the service life of concrete exposed to complex environments.

2. Experimental

2.1. Raw materials and mixing ratio

In this experiment, 42.5# ordinary Portland cement (OPC) with C_3A, C_4AF, C_2S, and C_3S content of 7.4%, 8.9%, 18.1%, and 60.5%, respectively, was used. The microsilica fume comprised more than 90% SiO_2 with average diameter of 0.31 µm. The superplasticizer had a water-reducing rate of 29% and a solid content of 31%. The three diameter ranges of quartz sand particles were 0.160–0.315, 0.315–0.625, and 0.625–1.250 mm, with mixing ratio of 1:4:2. The tensile strength, diameter, and length of the short thin steel fibers were 2800 MPa, 0.22 mm, and 13 mm, respectively. The only mixing ratio of cement:quartz sand:silica fume:steel fiber:superplasticizer:water used in this experiment was1:1.77:0.23:0.23:0.11:0.17. The water to binder ratio was 0.20, and the volume fraction of steel fibers was 2.0%. Table 1 lists the main performance of reactive powder concrete.

2.2. Experimental method

Molds of the formed samples were removed after 24 h of curing at room temperature. Then, the samples were placed in a steam-curing box at 75 °C for another 72 h of curing; the heating and cooling rates were both maintained at 15 °C/h. The samples were finally placed and stored in a standard curing room (T = 20 °C and RH greater than 95%) for up to 28 days. An NaCl solution (5.0 wt%) was used as the medium for the freeze–thaw cycling tests; the circulation mechanism implemented was identical to that described in China's National Standards for Testing Methods [13]. In a single freeze–thaw cycle, the temperature at the sample center decreased from 5 ± 2 °C to −18 ± 2 °C before increasing to 5 ± 2 °C within a span of 2–4 h, and the cycle time is 3 h in this experiment. The concrete sample had dimensions of 100 × 100 × 100 mm^3. Samples for chloride ion concentration testing were extracted at the following depths with respect to the specimen surface: 0–5, 5–10, 10–15, 15–20, 20–25, and 25–30 mm, as shown in Fig. 1. The extractions were performed after 200, 400, 600, 800, 1000, 1200, 1400, and 1500 freeze–thaw cycles. The chloride ion concentrations (mg/g; ratio of chloride ion mass to total cementitious material content) were evaluated by using a CLC-AL-type rapid chloride ion concentration tester.

To better understand the influence of freeze–thaw cycling on chloride ion diffusion, a natural soaking experiment was designed. For this test, specimens were immersed in the solution at room temperature until the time of testing. The testing solution and chloride ion concentration testing method were identical to those used in the freeze–thaw cycles; evaluations were performed after 30, 60, 120, 180, 360, 540, and 720 days of soaking.

2.3. Results of chloride ion concentration experiments

Table 2 shows the chloride ion concentrations of reactive powder concrete after freeze–thaw cycling and natural soaking. The chloride ion concentrations increased significantly after 1000 cycles, and the chloride ion concentrations of samples extracted at depths exceeding 15 mm were less than 0.2 mg/g. The chloride ion concentrations at the concrete surface after natural soaking were considerably higher than those obtained below the surface. Additionally, at depth of 10–30 mm, the chloride ion concentrations were nearly 0 mg/g. The chloride ion concentrations increased with the duration of natural soaking; the surface chloride ion concentration after soaking for 720 days was nearly six times that of samples soaked for 180 days. Because the indoor freeze–thaw cycling experiment was performed eight times per day, the number of days could be determined from the number of cycles. The chloride ion concentration of specimens after 1500 cycles (equivalent to 187.5 days) was the highest, and that of specimens after a similar duration of natural soaking (180 days) was much lower than those of specimens that underwent freeze–thaw cycling. Thus, freeze–thaw cycling accelerates chloride ion diffusion in concrete.

3. Chloride ion diffusion coefficients

3.1. Chloride ion diffusion coefficients for natural soaking

Natural chloride diffusion in ordinary concrete could be described by Fick's second law as follows.

$$c(x,t) = c_s\left(1 - erf\left(\frac{x}{2\sqrt{Dt}}\right)\right) \quad (1)$$

Table 1
Main performance of reactive powder concrete.

Performance	Compressive strength	Flexural strength	Splitting tensile strength	Fracture energy	Porosity
Specimen size (mm^3)	100 × 100 × 100	100 × 100 × 400	100 × 100 × 100	100 × 100 × 400	2–5 in diameter
Value	150.1 MPa	25.2 MPa	14.8 MPa	6.36 kJ/m^2	5.70%