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A numerical algorithm for evaluating the chloride diffusion coefficient of concrete with crushed aggregates

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HIGHLIGHTS

- The chloride diffusion coefficient of concrete with crushed aggregates is evaluated.
- The distribution of polygonal aggregates is simulated within a square element.
- The validity of the numerical method is verified with two sets of experimental data.

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ABSTRACT

Since the deterioration of marine reinforced concrete structures is, to a great extent, related to the movement rate of chloride ions in concrete, it is essential to determine the chloride diffusion coefficient of concrete through experiment or theoretical prediction. This paper proposes a numerical algorithm for evaluating the chloride diffusion coefficient of concrete with crushed aggregates. In the numerical algorithm, the mesostructure of three-phase concrete is reconstructed by generating polygonal aggregates of various sizes and placing them within a simulation element with periodic boundary conditions. The random walk algorithm is then applied to the simulated three-phase concrete for computing the chloride diffusion coefficient. With this algorithm, the reasonable values of the random walk radius and the number of simulations are determined. Finally, comparisons are made between the calculation results and the experimental ones obtained from the literature to verify the numerical algorithm. Based on several numerical examples, three primary factors, the aggregate content, and the thickness and chloride diffusion coefficient of interfacial transition zone, influencing the chloride diffusion coefficient of concrete, are evaluated quantitatively. This paper concludes that the proposed numerical algorithm is effective in evaluating the chloride diffusion coefficient of concrete with crushed aggregates.

1. Introduction

It has been recognized from laboratory experiments and field observations that reinforcement corrosion due to the penetration of chloride ions is the primary cause accounting for the cracking, spalling, and even delaminating of reinforced concrete (RC) structures exposed to chloride environments. In the past thirty years, lots of such cases were reported around the world, such as major spalling in bridge decks [1], significant corrosion in jetty substructures [2], and severe surface cracking of concrete buildings [3]. Therefore, it is important to measure or predict the transport properties of concrete and to analyze the primary influential factors for the service life estimation and durability design of RC structures [4].

On the experimental side, Delagrave et al. [4] adopted two methods to test three series of mortars and found that sand modifies the microstructure by forming a porous interfacial transition zone (ITZ) on the surface. This is due to the fact that cement is a particulate material with a mean size around 10 μm, while the aggregate diameter is at least 0.15 mm in normal concrete. When encountering the much larger aggregate, the cement grains are subjected to the "packing" constraints imposed by the aggregate surface, resulting in a local increase in porosity. The overall effect of the ITZ, tortuosity, and dilution induced by the addition of sand particles leads to a decrease in chloride diffusion coefficient. However, Halamickova et al. [5] and Asbridge et al. [6] also showed that the ITZ becomes percolating once the sand content reaches a

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critical value, leading to an increase in chloride diffusion coefficient. Yang and Su [7] applied a migration test to estimate the transport properties of mortar and evaluated the effect of the aggregate content on the chloride diffusion coefficient. Based on experimental results, Caré [8] quantified the competing effects of the ITZ and the tortuosity and concluded that addition of aggregates results in a denser cement paste and hence a smaller chloride diffusion coefficient.

On the theoretical side, various effective medium approximations and numerical techniques are used to analyze the chloride regress into cementitious materials. By introducing the concept of ITZ percolation and modeling mortar as an ordered periodic aggregate geometry, Garboczi et al. [9] expressed the chloride diffusion coefficient as a function of those of ITZ and cement paste. For low aggregate content concrete, the chloride diffusion coefficient and other properties were derived analytically [10]. By considering the characteristics of three phases in concrete, Caré and Herve [11] formulated the chloride diffusion coefficient. Zheng et al. [12] developed a semi-empirical, three-phase composite sphere model to evaluate the effect of the ITZ on the chloride diffusion coefficient of concrete. Aggregate shape was also shown to exert a certain influence on the transport coefficient of concrete [13]. Sun et al. [14] presented a multi-scale method to evaluate the chloride diffusion coefficient of concrete and analyzed the main influential factors. Šavija et al. [15] developed a lattice model to simulate the transport of chloride ions in sound and cracked concrete. With the ionic binding effect, Liu et al. [16] presented a two-dimensional, multi-component model for the ionic transport in concrete. Besides the ITZ and aggregate, they also evaluated the effect of ionic binding on the chloride diffusion coefficient. Li et al. [17] introduced the concept of double porosity to describe the ingress of chloride ions into concrete. Du et al. [18] evaluated the effects of various mesotructural parameters on the chloride diffusion coefficient of concrete. However, in the above-mentioned analytical methods, aggregates are all assumed to be spherical (circular) or ellipsoidal (elliptical) and hence they are not appropriate for concrete with crushed aggregates. In these numerical methods, heterogeneous concrete is reconstructed and the governing differential equations have to be solved for different random configurations, which proves to be time-consuming [19]. It is therefore essential to present an efficient numerical algorithm for estimating the chloride diffusion coefficient of concrete with crushed aggregates.

This paper presents a numerical algorithm for simulating the mesostructure of concrete with crushed aggregates and for evaluating the chloride diffusion coefficient. In placing polygonal aggregates into a square element, periodic boundary conditions are introduced to avoid artificial wall effects. Based on the simulated mesostructure, the random walk method is applied to the computation of the chloride diffusion coefficient. Comparisons with experimental results verify the validity of the numerical algorithm and numerical examples are given to quantify the main influential factors.

2. Mesostructural simulation of concrete with polygonal aggregates

At present, it is still difficult to simulate the mesostructure of concrete with polyhedral aggregates. For this reason, the random walk algorithm is limited to two-dimensional concrete with polygonal aggregates in this paper. Thus, aggregates are modeled as convex polygons and randomly distributed in the cement paste. For a convex polygonal aggregate, the diameter d is defined as the smallest width of all excribed rectangules which are just big enough to contain the particle wholly inside. From the sieve analysis, the aggregate size distribution can be expressed, with respect to the number of aggregates, by a cumulative distribution function $P(d)$ [20]. For the purpose of computer simulations, an element with sizes of $a \times a$ is chosen. When the aggregate area fraction f_a, which is defined as the area ratio of all the aggregates to the simulation element, is given, the computer simulation procedure consists of the generation and distribution of aggregates.

For convenience, W is defined as a random variable uniformly distributed on the interval (0, 1). The aggregates conformed to $P(d)$ are generated as follows:

1. In general, the number of sides of a crushed aggregate is between 3 and 10 [21]. If there is no further information on this parameter, the number of sides m_i of the i-th aggregate may be taken as a random integer variable uniformly distributed between 3 and 10, i.e.,
$$m_i = [3 + 8w_{i1}] \tag{1}$$
where w_{i1} is sampled from W and $[x]$ denotes the largest integer smaller than or equal to x.
2. In the polar coordinate system, the j-th polar angle θ_j $(j = 1, 2, \ldots, m_i)$ of the aggregate can be obtained as
$$\theta_j = 2\pi w_{j2} \tag{2}$$
where w_{j2} is sampled from W. The polar angles are rearranged from the smallest to the largest. If the elongation ratio is controlled to vary randomly between A_1 and A_2, the corresponding polar radius r_j is given by
$$r_j = A_1 + (A_2 - A_1)w_{j3} \tag{3}$$
where w_{j3} is sampled from W.
3. If the aggregate is concave, the coordinates are all invalid and need to be regenerated by returning to step 2 until it becomes convex.
4. The diameter d_i of the aggregate is given by solving the following equation
$$P(d_i) = w_{i4} \tag{4}$$
where w_{i4} is sampled from W. The aggregate is then enlarged or shrunk in all directions so that the diameter is equal to d_i exactly. The area s_i is calculated and added up to the total area S_i of i aggregates that have been generated so far, using
$$S_i = S_{(i-1)} + s_i \tag{5}$$

If $S_i \geqslant f_a a^2$, stop the aggregate generation, and the number of aggregates N_a is equal to i. Otherwise, repeat steps 1 to 4 until $S_i \geqslant f_a a^2$.

When these generated aggregates are placed within the simulation element, a periodic boundary condition is introduced to avoid any wall effects. The details are as follows:

1. The aggregates are rearranged from the largest to the smallest.
2. The center coordinates (x_i, y_i) of the i-th aggregate $(i = 1, \ldots, N_a)$ are determined by
$$x_i = aw_{i5}, \quad y_i = aw_{i6} \tag{6}$$
where w_{i5} and w_{i6} are both sampled from W. The aggregate (in black) will be situated completely within the element Fig. 1(a) or extend beyond the element Fig. 1(b) and (c).
3. If the aggregate extends beyond the element, additional aggregates (in grey) are generated at a distance of a from the aggregate in the two directions, as shown in Fig. 1(b) and (c).
4. If the newly placed aggregates do not overlap with those already placed, repeat steps 2 and 3 for the next aggregate.