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Effects of crack and ITZ and aggregate on carbonation penetration based on 3D micro X-ray CT microstructure evolution

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HIGHLIGHTS

- Carbonation depth of cement mortar with different BFS are monitored by in situ X-ray CT.
- Effects of crack width and length on carbonation penetration are analyzed.
- Effects of ITZ diffusivity and thickness on the diffusivity of carbon dioxide are researched.
- Effects of aggregate size and content on the diffusivity of carbon dioxide are researched.

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ABSTRACT

Previous researchers have made a lot of contributions on carbonation reaction. However, effects of multi-cracks and interfacial transition zone (ITZ) on the diffusivity of carbon dioxide are critical and thorny problems. In this study, numerical simulation of carbonation process using the COMSOL Multiphysics are presented based on in-situ 3D microstructure evolution of X-ray CT. Firstly, micro X-ray computed tomography (X-ray CT) was used to monitor the carbonation depth evolution of cement mortar with different additions of blast furnace slag (BFS). It is shown that the optimal addition of blast furnace slag (BFS) against the carbonation is no more than 50%. In addition, COMSOL Multiphysics numerical model based on micro X-ray CT image was used to investigate effects of transverse crack and interfacial transition zone (ITZ) on the diffusivity of carbon dioxide. Finally, effects of different crack width, length, ITZ of polygon Random Aggregate Structure (RAS), and aggregate size and content on the diffusivity of carbon dioxide have been investigated.

1. Introduction

In recent years, the concentration of carbon dioxide gas in the atmosphere increase significantly. The increase of carbon dioxide concentration and higher temperature due to green-house effect have greatly accelerate the carbonation reaction rate of reinforced concrete. Carbonation reaction will lead to the corrosion of steel bar and reduce the durability of reinforced concrete [1]. Carbonation is one of the most serious durability problems which have a great impact on the service life of engineering structure. The former researchers have been a lot of important contributions, i.e. carbonation chemical mechanisms [2–6], carbon dioxide diffusivity [7–9], microstructure changes [10–13], etc.

However, effects of multi-cracks and interfacial transition zone (ITZ) on the diffusivity of carbon dioxide are critical and thorny problems. Schutter et al. [14] investigated the effects of existing cracks in mortar specimens on the carbonation and chloride penetration, a formula with crack width and crack length was proposed to qualify the influence of the cracks. Liang et al. [15] established a carbonation model for concrete with cracks and predicted the carbonation depth in cracked concrete by using a statistic method. By the use of 100% CO_2 accelerate test and a linear, least squares best fit analysis, Green et al. [16] found that there is 67% confidence that carbonation penetration varies with the change of crack width. Alahmad et al. [17] studied the carbonation penetration on mortar with both artificial cracks (sawed specimens) and real cracks controlled by means of a mechanical expansive core. Their experimental results showed that there exist two thresholds of crack width for the perpendicular-to-crack wall carbonation penetration. The perpendicular-to-crack carbonation depth is close to the surface carbonation depth when the crack width is not less than 60 μm, but for crack width less than 9 μm, the perpendicular-to-crack carbonation can hardly be observed. In addition, they found that

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the perpendicular-to-crack carbonation depth similar to surface carbonation depth no matter the variations of crack width, this may due to lacking of an interlocking phenomenon between the fractures surfaces in artificial cracks which can reduce the CO_2 diffuse capability in real cracks.

Recently, several studies on ITZ properties have been conducted. Jin et al. [18] found that the diffusivity of ITZ and aggregate content have a notable effect on chloride penetration in concrete while aggregate shape and aggregate distribution have a negligible impact on chloride attack. Bernard et al. [19] investigated the influence of ITZ on the diffusivity as well as on its mechanical properties by using 3D MUMOCC platform (Multiscale Modeling of Computational Concrete), they found that there was slight effect of ITZ on diffusivity because the porosity of paste and ITZ balance each other. Larrard et al. [20] investigated the effects of the shape of coarse aggregates on the macroscopic drying and carbonation phenomena in concrete by means of 3D FE simulations. Nobuaki et al. [21] studied the influence of recycled aggregate on ITZ, carbonation and chloride ingression of concrete. It is shown that double mixing could improve the ITZ properties and decrease the carbonation depth. However, it did not consider the effect of ITZ properties on concrete carbonation progress. Meanwhile, the aggregate shape almost assumed to be circular without considering the real aggregate shape (polygon) in previous simulation investigations. In addition, little research has been devoted on meso-scale modeling of concrete carbonation.

X-ray computed tomography (X-ray CT) and COMSOL Multiphysics simulation are excellent methods because it can provide a noninvasive and nondestructive method to obtain 3D microstructure information of cement based materials without any prior specimen preparation. X-ray computed tomography also has been applied by various researchers in carbonation reaction [22–24]. Previous researchers have used the COMSOL Multiphysics simulation to model cracks and chloride transport properties [25–26].

In this study, numerical simulation of carbonation process using the COMSOL Multiphysics are presented based on in-situ microstructure evolution of X-ray CT. Firstly, micro X-ray computed tomography (X-ray CT) have been monitored the carbonation depth evolution of cement mortar with different additions of blast furnace slag (BFS). In addition, COMSOL Multiphysics numerical model based on micro X-ray CT image based microstructure was used to investigate effects of transverse crack and interfacial transition zone (ITZ) on the diffusivity of carbon dioxide.

2. In-situ microstructure evolution of X-ray CT

2.1. Raw materials

The cement used is Portland cement (PC, strength class 52.5 N/mm^2, produced in Huaxin, fineness: 350 m^2/kg), with the chemical and mineral composition listed in Table 1. The chemical composition of blast furnace slag is shown in Table 2.

Table 2
Chemical composition of blast furnace slag.

CaO	SiO_2	Al_2O_3	Fe_2O_3	MgO	SO_3	K_2O	Na_2O	Others
34.54%	34.86%	16.97%	1.12%	6.90%	1.65%	0.45%	0.46%	3.05%

2.2. Carbonation sample preparation

Some cylindrical samples (diameter 46.1 mm, length 72.8 mm) of mortar with blast furnace slag were prepared for the experiments. The water to cement ratio was 0.53 and the sand to cement ratio was 2.0. The replaced fractions by weight of Portland cement with blast furnace slag were 0%, 30%, 50% and 70%. Some cylindrical polyvinyl chloride tubes were sealed by adhesive tape for early hydration and hardening period. The mixture of cement, blast furnace slag, sand and tap water were injected into cylindrical polyvinyl chloride tubes and vibrated for 10 s to reduce voids using a bench-top vibrating table. The samples were rotated with rotate bed for 24 h to reduce bleeding or segregation. Afterwards, the specimens were stored in standard curing room at 20 ± 3 °C for 3 months. After curing, the polyvinyl chloride tube was removed, and the specimen was dried at 50 °C in the oven for 48 h. After sealing the top and bottom surfaces with hot paraffin, the specimen was transferred to a carbonation chamber with a CO_2 concentration 20 ± 3%, RH 70 ± 5%, and Temperature 20 ± 2 °C.

2.3. Image based microstructures evolution

Micro X-ray computed tomography (X-ray CT) have been monitored the carbonation depth evolution of cement mortar with different additions (0%, 30%, 50% and 70%) of blast furnace slag (BFS), respectively. The evolution of carbonation front depth have been monitored in-situ by Micro X-ray computed tomography (X-ray CT) at different accelerated carbonation ages, 0 days, 3 days, 7 days and 14 days, respectively.

The specimens were scanned with an YXLON micro-focus X-ray CT system (Y. CT Precision S, YXLON). XCT is a three-dimensional imaging technique that uses a series of radiographic images to reconstruct a map of an object's X-ray absorption. A principle illustration of the computed tomography system used in this work is shown in Fig. 1.

The voltage and current of the X-ray tube were 195 kV and 0.35 mA, respectively. The type of detector was Y. XRD 0820 with 1024 detector elements, and the number of actual detector pixels was 1024. The cone beam magnification (object center) was 3.01 times. The number of projections was 1080, and the object rotation angles were 360°. The filter is composed of sternums sheets (Sn, 0.50 mm). The 2D pixel size (minimum resolution) was 0.066 mm × 0.066 mm. The 3D voxel size (minimum resolution) was 0.066 mm × 0.066 mm × 0.066 mm.

The micro X-ray CT images are spatial distribution of the linear attenuation coefficients expressed by gray values, meanwhile, the higher density zone with brighter area corresponding to the higher values of linear attenuation coefficients, and the lower density zone with darker zone corresponding to the lower values of linear

Table 1
Chemical and mineral composition of the Portland cement 52.5.

CaO	SiO_2	Al_2O_3	Fe_2O_3	MgO	K_2O	TiO_2	MnO	SO_3	Na_2O	Insol.	LOI
62.60%	21.35%	4.67%	3.31%	3.08%	0.54%	0.27%	0.18%	2.25%	0.21%	0.59%	0.95%
C_3S		C_2S		C_4AF		C_3A		$C\overline{S}H_2$		Others	
55.5%		19.1%		10.1%		6.5%		5%		3.8%	

Insol.: insoluble residue. LOI: loss on ignition.