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Carbonation modeling analysis on carbonation behavior of sand autoclaved aerated concrete

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HIGHLIGHTS

- The compressive strength of SAAC decreased with the increase of carbonation depth.
- Phase component and microstructure significantly changed with the increase of carbonation depth.
- An appropriate value of the carbonated substance reaction coefficient based on experimental results was proposed for SAAC.
- A practicable mathematical model displays a high potential for the estimations of carbonation rate in SAAC.

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ABSTRACT

Carbonation could not be ignored because of the significant deterioration of mechanical property and durability of sand autoclaved aerated concrete (SAAC). A better understanding and quantification are necessary for maintaining and repairing the existing structures of SAAC. A practicable mathematical model based on the Fick's first law was established, which was evaluated by the data of accelerated carbonation experiment. Carbonation behavior was studied by means of phenolphthalein test, SEM and XRD. Because the tobermorite generated by hydration gradually transformed into calcite, the compressive strength of samples showed an obvious decline with carbonation depth increased. Furthermore, the experimental date of B05 bulk density class SAAC samples and the calculated values of model have shown good agreements.

1. Introduction

Sand autoclaved aerated concrete (SAAC) is a typical kind of cellular material, which commonly manufactured by steam curing [1]. The raw materials contain cement, lime, gypsum, water and aluminum powder, which acts as a pore forming agent [2–4]. Due to using quartz sand as the siliceous raw material, the properties of SAAC is different from Fly ash autoclaved aerated concrete (FAAC), such as a relatively strength-volume density, lower drying shrinkage and better insulation performance of SAAC. For the advantages of lightweight, excellent thermal insulation ability, appropriate strength and good construction, SAAC is widely used as a wall material in many countries [5,6]. When more and more attention has been paid to building energy conservation [7,8], SAAC with good thermal insulation property is used as the only one type of wall materials which meet the requirement of 50% of the building energy conservation in Chinese national standard [9].

Over the past decades, some studies have showed that the carbonation of autoclaved aerated concrete results in the degradations of structures, such as the changes of minerals and microstructures, mechanical properties falling, cracking and the increase of drying shrinkage [10,11]. Moreover, carbonation of autoclaved aerated concrete can accelerate ageing of the coating on steel bars, leading to steel corrosion and structural failure [12]. As exposing to the air, the aging deterioration possibly affects the durability and service life of autoclaved aerated concrete in general.

Carbonation of concrete is the reaction between the calcium-based phases and carbon dioxide from the air, which enters the concrete via the pore network [13]. For FAAC, carbonation is the chemical reaction between the main structural minerals and carbon dioxide [14], where 1.1 nm-tobermorite and well-crystallized calcium silicate hydrate react with carbon dioxide either dissolved in water or gas under the existence of moisture and finally decomposed to silica gels and calcium carbonate. The main chemical reactions are described detailedly in previous studies [11,15].

With the carbonation process going on, the mechanical properties and durability of autoclaved aerated concrete significantly

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declined due to the change of major mineral crystals [16,17]. However, it is not easy to observe the microcosmic changes in engineering conditions.

Carbonation depth is a key parameter in the investigation of the service life of reinforced concrete structures and can well characterize carbonation rate. The distance between the exposed surface of the sample and the carbonation front can help designers to determine the thickness of the concrete cover to protect reinforcement bars from corrosion [18]. Carbonation modeling for ordinary concrete has been a research hotspot and a lot of available carbonation models based on the mass conservation law and Fick's first law have been developed. These models can be divided into different categories: empirical models, statistical models, numerical models, simulation models [19,20]. Most of models in the literatures are experiential, and their mathematical expressions relate the carbonation depth d with the square root of time t as follows:

$$d = k \times \sqrt{t} \quad (1)$$

where: k is the carbonation rate and it depends on the surrounding conditions and the properties of the concrete. To identify the parameter k, a constitutive relation between relative humidity, porosity changes and diffusivity of carbon dioxide during carbonation is parameterized. However, these empirical models may be not applicable for autoclaved aerated concrete. Because the raw materials are not all the same or physical and mechanical properties are significantly different. For example, there is no coarse aggregate in autoclaved aerated concrete, the raw materials are compounded as slurry. Similarly, the porosity of autoclaved aerated concrete can vary from 60% to 80% which is much higher than that of ordinary concrete [21].

Mathematical models might have potentiality to validate or develop for SAAC. An analytical model which calculates the change of bulk density has been developed by Hanecka [22]. Some researchers proposed the ratio of compressive strength before and after carbonation as a criterion for the degree of carbonation in fly ash autoclaved aerated concrete (FAAC) [23]. The XRD peak intensities of 1.1 nm-tobermorite were used as a criterion for carbonation. Furthermore, the amounts of carbon dioxide adsorption were used to investigate carbonation degree of FAAC [24]. However, the bulk density and compressive strength vary with the moisture content, and the criterion of micro level do not quite convenient in a practical project.

The accelerated carbonation tests for B05 bulk density class SAAC were carried out. The relation between compressive strength and carbonation depth was investigated during the carbonation process. The microcosmic changes of carbonated samples were observed by means of SEM and XRD. Then, a practicable model to calculate carbonation depth under the carbonation process was developed in this article. Some influencing factors were taken into account, such as bulk density and relative humidity. Finally, modified model was validated with experimental data and an appropriate value of the carbonated substance reaction coefficient for SAAC was proposed.

2. Materials and experiment

2.1. Materials

The B05 SAAC samples were provided by Shanxi Ningyuan New Wall Materials Co. Ltd. The product numbers of B05 indicates an approximate nominal apparent density of 500 kg/m^3. The chemical composition of the chief raw materials and compositions of SAAC forming mixture were presented in Tables 1 and 2, respectively. All of the samples were cut into cube having dimensions of 100 × 100 × 100 mm^3. Before artificial weathering, the specimens were dried to the objective moisture contents (10%) in drying oven at 105 ± 5 °C, laying up some soda lime in drying oven to ensure the cubes not to be carbonized. Then five faces of each specimen were sealed with paraffin and actualized one-dimensional carbonation.

Table 1
Chemical compositions of the main raw materials (in mass%).

Composition	SiO_2	Al_2O_3	Fe_2O_3	CaO	MgO	LOI
Sand	85.94	6.48	0.39	1.97	0.46	4.76
Cement	20.88	5.96	4.55	62.80	1.03	4.78
Lime	3.75	1.81	0.68	90.46	2.26	1.04

Table 2
Mix proportions of raw materials for SAAC (wt%).

Composition	Sand	Cement	Lime	Gypsum	Al powder	Water/solid
B05	62.0	18.0	18.0	2.0	0.085	0.61

2.2. Methods

As carbonation of cement-based materials under nature conditions is a slow process [20,25], high carbon dioxide concentration in carbonation conditions can accelerate the carbonation rates. Therefore, the accelerated carbonation test was carried out. The accelerated groups were performed in the chamber at 20% carbon dioxide concentration, 20 ± 2 °C temperature and relative humidity 55 ± 5%.

2.2.1. Evaluation of carbonation depth and compressive strength

The carbonation depths of SAAC specimens were measured by the conventional method of chemical reagent at different carbonation periods. Firstly, specimens were cut into two parts perpendicular to exposed surfaces with a saw. Then 1% Phenolphthalein alcohol solution was sprayed on split surface to observe the variation of the color. Finally, different measuring points were chosen to determine the carbonation depth with a vernier caliper and calculated the average value.

The porosity was determined the bulk density and matrix density of samples at dry state. The bulk density was measured by Archimedes's displacement principle, while the matrix density was measured by pycnometry.

The samples were dried before the compressive strength test, most of paraffin was melted and a blade was used to scrape the residual paraffin. Then, the compressive strength was conducted using a powerful electromechanical testing machine at loading rate of 2.0 ± 0.5 kN/s according to GB/T 11969-2008 "Test methods of autoclaved aerated concrete".

2.2.2. Evaluation of microstructure

Phase compositions of SAAC samples were investigated by X-ray diffraction (XRD) before and after carbonation. The microstructural difference between carbonated and non-carbonated samples was observed using scanning electron microscopy (SEM).

3. Results and discussion

3.1. Carbonation rates

The average values of carbonation depth and porosity for B05 bulk density class SAAC samples at different carbonation ages exposed to the artificial condition are shown in Table 3. Due to the transient exposure to ambient air can be neglected, the initial carbonation depths are assumed to be zero at the beginning of carbonation test. Moreover, due to the limit of dimension for samples, the carbonation depth may be bigger than 100 mm at 96 h.

As presented in Table 3, carbonation process of SAAC was so rapid that all the specimens were completely carbonized at 96 h. The carbonation depths of SAAC were more than ten times that observed in ordinary concrete, which about 7 mm of ordinary con-

Table 3
Average carbonation depth and porosity in artificial condition.

Time (h)	0	4	8	16	32	48	96
Depth (mm)	0	19	31	50	70	85	100[a]
Porosity (%)	75.71	75.63	75.56	75.50	75.41	75.33	75.22

[a] The B05 SAAC samples were completely carbonized at 96 h, namely carbonation depth ≥ 100 mm.