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Coupling effect of temperature and relative humidity diffusion in concrete under ambient conditions

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HIGHLIGHTS

- An improved microstructural hydration model.
- An integration of hydration model to moisture and temperature transfer in concrete.
- A water content redistribution into pores of concrete based on adsorption effect.
- A engineering project verification of the model under ambient conditions for a long time.

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ABSTRACT

To accurately analyze the temperature and relative humidity (RH) distribution in concrete structures under ambient conditions, based on Krstulovic-Dabic hydration kinetics, an improved hydration model is proposed to geometrically bridge the relationship between hydration degree and microstructure of cementitious materials. Both the water content and hydration heat can be individually extracted from the model to evaluate the influence of ambient conditions variation. And the adsorption curve of concrete is acquired based on the microstructure obtained from hydration model and a redistribution of moisture content in pores is applied to evaluate the hydration process accordingly. Thus, the coupling effect of RH and temperature diffusion in concrete is decoupled in terms of hydration degree. An engineering verification indicates that the model can accurately predict the development of relative and temperature in concrete structures, and the construction procedure has significant influence on moisture and heat diffusion in concrete under ambient conditions.

1. Introduction

The durability of concrete structures is now widely accepted to be a very important property of concrete structures, which is of remarkable significance for their service performance during the whole life cycle. To a great extent, it is recognized that the durability of concrete structures depends on the volume stability, or in other words deformation of concrete [1]. Generally, there are two kinds of deformation of concrete, power deformations due to applied external load and own deformation caused by changes of temperature and moisture content, such as shrinkage and creep [2]. A statistical analysis indicates that only 20% of concrete cracks are induced by so-called applied external loads consisting static, dynamic loads and so on Ref. [3]. Correspondingly, the own deformation of concrete is far more important for the durability of structures, especially under constantly changing ambient conditions.

As the ambient environments are generally believed to be one of the most important factors that will cause durability deterioration of concrete structures, the behaviors of concrete under ambient conditions have drawn more and more attentions in last decades [4–6]. Among all the ambient effects, temperature and humidity variation are the most common ambient actions, which can change dramatically during the lifetime of a structure. In comparison with the seasonal variations, a sudden change of ambient actions, including rainstorm, dense fog, heavy frost, strong sunshine and so on, will cause a noticeable response on the volume stability of concrete, then furtherly affect the internal stress distribution of concrete structures [7]. Such actions are important not only during the service period but also during the construction period for a concrete structure. In construction stage, especially at the early-age, the behaviors of concrete structure are more sensitive to temperature and humidity variations as they will influence heat release and water consumption process induced by cement hydration. Furthermore, the construction technologies and procedures have a major impact on the surficial environmental conditions of

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a structure, such as demolding, curing, coating, surface decoration, etc. From this perspective, both the natural and the artificial ambient actions, from construction to operation, account for the durability of a structure [8].

Based on classical phenomenological theory, many scholars studied the heat and mass transfer concerning thermo-hygro coupling [9]. While in this research, the transfer parameters calculation can not reflect the essence of coupling effect. In 2006, the hybrid mixture theory considering the characteristic of the microstructure evolution of early-age concrete was employed to establish the coupling model proposed by Gawin et al. [10], in which the moisture transfer in concrete was divided into the transport of water vapor and capillary water separately. Based on the work of Gawin et al., the influence of concrete pore structure on moisture transfer was taken into account in an improved model established by Du et al. [11]. Furthermore, a fully coupled and non-linear formula was designed to predict the behavior and potential for spalling of heated concrete structures induced by the coupling effect of heat and moisture for fire and nuclear reactor applications [12,13]. Although a simplified coupled thermo-hydro-mechanical model was developed to analyze the damage of concrete subjected to moderate temperatures, but this research still focused on concrete behaviors under relatively high temperature which cannot be applied to ambient conditions analysis [14]. The similar research under ambient temperature was still rare.

By now, the investigations for coupled thermos-hygro behaviors of concrete emphasize on either early-age or hardened concrete. Rare studies can efficiently bridge the long-term heat and moisture diffusion with hydration process of concrete by considering the microstructure evolution and permeability development. Under changeable ambient conditions, the saturation of concrete remarkably depends on the moisture diffusion history which should be traced back step by step to construction process of a structure. Moreover, the ultimate hydration degree in concrete is determined not only by the water to cement ratio but also by the varying history of ambient temperature and relative humidity (RH). Thus, to accurately predict the long-term behaviors, the model must account for variation in the temperature and moisture states from construction to operation of a concrete structure.

In this research, a microstructure hydration model is proposed to demonstrate the microstructure evolution and the hydration progress of concrete. The hydration heat and moisture consumption obtained from the hydration model are employed in Fourier equations to describe the coupling effect between moisture transport and heat transfer in concrete. The ambient actions history is considered in the thermo-hygro coupling model to simulate the development of RH and temperature in concrete structures. And the model is furtherly validated in an engineering practice.

2. An improved cement hydration model

2.1. Basic hydration unit

Briefly, the cement hydration process can be taken as a series of chemical and physical reactions between cement particles and the water around them. Through chemical reactions, the chemical energy contained in cement particles will be released in terms of hydration heat. According to the principle of minimum potential energy, the stable state can only be achieved when the chemical potential gets to the lowest level. So, the hydration process will not stop when the cement particles are in appropriate micro-environmental conditions. Therefore, the chemical reactions are the inner driven force for cement hydration. At the same time, the hydration products generation and water depletion also physically change the micro-environment around cement particles. The reduction of water pressure and the engulfment of cement particles will gradually retard the hydration process. Hence, both the chemical and physical reactions during cement hydration should be taken into consideration in the cement hydration model.

In this research, an improved hydration model is established based on the study of Tian et al. [15,16]. For sake of simplicity, all cement particles are assumed to be spherical. In Tian's model, it is suggested that all the cement particles dispersed in water do not contact with each other at the beginning of hydration. As shown in Fig. 1, each particle and corresponding water is geometrically formed in a cubic lattice and the entire hydration reactions is assumed to perform within this lattice. Because the hydration of a cement system consists of the hydration of cement particles in these lattices, the lattice can be stated as the basic hydration unit in this research.

In this research, the side length of the basic hydration unit containing a cement particle with the initial radius R at time t is denoted as $L_R(t)$. The initial volume of a basic hydration unit depends on water to cement ratio and the radius of cement particle, and the initial side length, $L_R(0)$, can be calculated mathematically as:

$$L_R(0) = \left[\frac{4\pi}{3}(\rho_{cw}w_0 + 1)\right]^{1/3} R \quad (1)$$

where ρ_{cw} is specific gravity of cement; w_0 is water to cement ratio; R stresses the initial radius of cement particle in the basic hydration unit.

In comparison with Tian's model, the rigid boundary of the basic hydration unit is replaced by a permeable membrane on the faces of the lattice, which means that not only the hydration heat but also the liquid phase can flow across it. As a result, the moisture content is also extracted from the model as well as the hydration heat. Thus, the improved hydration model can be used to analyze both the heat and moisture transfer in concrete regarding the ambient conditions. But the solid phase, such as the hydration products, is assumed to be blocked by the membrane which cannot penetrate through the membrane.

2.2. Microstructural hydration model

2.2.1. Microstructural model of hydrated cement particle

In basic hydration unit, the cement particle submerges in water and the chemical reactions naturally proceed from the surface to its inside. And the hydration products will finally deposit on the surface of the cement particle. As shown in Fig. 1, a hydrated cement particle in the basic hydration unit is composed of three parts, the outer hydration products layer, the inner hydration products layer and the unhydrated cement particle. With the development of hydration process, the radius of unhydrated cement particle continually decreases and the outer boundary of outer hydrated products layer increasingly expands. As demonstrated in Fig. 1, the inner radius, $R_{in,R}(t)$, represents the radius of unhydrated cement particle at time t. Accordingly, the outer radius, $R_{out,R}(t)$, indicates the outer boundary of the hydration products growing on the cement particle at time t. The geometrical parameters, L_R, $R_{in,R}$ and $R_{out,R}$, are essentially correlated with the hydration degree of the cement particle whose initial radius is R, as marked in the subscript. Then, the hydration process can be mathematically characterized by the variation of these parameters in the hydration model.

2.2.2. Hydration process of a single cement particle

Geometrically, the hydration of a cement particle in basic hydration unit is demonstrated in Fig. 2. Before hydration, as defined in Fig. 2(a), a cement particle is idealized as locating at

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