International Journal of Heat and Mass Transfer 115 (2017) 488–499

Contents lists available at ScienceDirect

International Journal of Heat and Mass Transfer

journal homepage: www.elsevier.com/locate/ijhmt

A hygro-thermo-chemical analysis of concrete at an early age and beyond under dry-wet conditions based on a fixed model

Wei Zhou, Tianqi Qi, Xinghong Liu *, Chuqiao Feng, Shuhan Yang

State Key Laboratory of Water Resources and Hydropower Engineering Science, Wuhan University, Wuhan 430072, China

ARTICLE INFO

Article history:
Received 27 March 2017
Received in revised form 16 July 2017
Accepted 6 August 2017

Keywords:
Hygro-thermo-chemical
Early-age and beyond
Fixed model
Dry-wet conditions

ABSTRACT

Based on a fixed hygro-thermo-chemical model that is clearly distinguishable from other models in the existing literature, this work conducts a finite element analysis of heat transfer and moisture transport for concrete at an early age and beyond. Numerical validations show that this fixed model corresponds to the hydration heat liberation rate for ordinary Portland cement and reflects the two-phase process of the relative humidity changes. Simulations of concrete samples with various water-cement ratios are performed, and the outcomes are compared to experimental temperature and relative humidity curves, confirming that the modified model has relatively high accuracy. The simulated influential depths of moisture transfer in concrete are also in accordance with the results from theoretical equations.

1. Introduction

The decreased structural performance of concrete during its service time is closely related to concrete cracking [1,2]. Study results indicate that shrinkage or expansion of concrete caused by changes in temperature and moisture is an important factor that influences cracking, particularly at an early age [3,4]. In the hydration process, the change in moisture in concrete is mainly influenced by self-desiccation and exchanges between concrete and the external environment. In turn, the variations in temperature and moisture commonly affect the hydration reaction [5]. Many studies have shown that environmental humidity variations cause an uneven distribution of moisture, which leads to a shrinkage gradient at the surface of the structure. Moreover, a low environmental humidity influences or even stops the normal hydration process due to moisture loss in the concrete, decreasing both concrete strength and durability [6-8]. Hydration behavior, self-desiccation, moisture exchange and cooling effects under external environmental conditions can produce temperature and moisture gradients in a concrete structure that may eventually lead to structural cracking [9-11]. Therefore, predicting the temperature levels, hydration behavior and moisture changes under various environmental conditions is of great significance for concrete structures.

The influence of temperature on the rate of hydration heat release follows the general chemical reaction law: as the temperature increases, the hydration reaction and the rate of hydration heat release accelerate. Temperature greatly affects the early hydration heat release rate of cement, but this effect gradually becomes smaller over time. Some studies have shown that [12] Portland cement can continue to hydrate at −5 °C but that hydration stops at less than −10 °C. In the hydration process at high temperature, the water in the system is rapidly consumed, and the unhydrated particles are encapsulated in the hydrated particles, increasing the diffusion and migration barrier. Thus, the hydration progress is greatly hindered, and the heat release rate of hydration substantially decreases. Studies have shown that [13] when the relative humidity of Portland cement is less than 0.8, the hydration reaction almost completely stops. Therefore, the moisture content in the system is an important factor affecting the hydration reaction process, which together determines the gelling material hydration rate and final degree of hydration with the temperature, heat and hydration degree.

Extensive experimental research and computational studies have sought to develop a general model for predicting the hydration heat and moisture change in concrete. The formulation of numerical hygro-thermo-chemical models has evolved over time. Ulm and Coussy proposed a thermo-chemo-mechanical model of early-age concrete based on the open porous media theory, and they introduced the hydration degree ξ to describe the hydration reaction of the cement and the mass of chemically bound water [14,15]. Cervera et al. proposed a coupled thermo-chemo-mechanical model for the behavior of early-age concrete that can be implemented in a finite element method to predict the evolution of the heat and degree of hydration over time [4,16]. Martinelli et al. proposed a complete theoretical formulation and an effective

* Corresponding author.
E-mail address: liuxht@126.com (X. Liu).

http://dx.doi.org/10.1016/j.ijheatmasstransfer.2017.08.014
0017-9310/

numerical implementation of a heat flow and hydration model for concrete hardening [17]. These studies and many other models of early-age concrete consider only thermo-chemical phenomena, neglecting the water diffusion process. However, this assumption is not always accurate, especially when moisture is exchanged between concrete and the external environment. Numerous efforts have been made to model the hygro-thermal behavior of concrete. For example, Bazant et al. proposed a phenomenological approach that is traditionally used in many studies, but they did not distinguish between the different phases of moisture [13,18]. Reference [19] added a sink term in the diffusion equation to account for endogenous drying in high strength concrete; however, that study did not consider the effect of hydration heat. Gawin et al. proposed a new numerical model that considered not only the thermal and chemical fields but also the water diffusion process [20]. DiLuzio et al. developed a complex model that considers the effect of the silica fume reaction and silicate polymerization [21]. Jendele et al. proposed a multiscale hydro-thermo-mechanical model for early-age and mature concrete that can be adapted to engineering analyses, but the moisture diffusion in the drying and wetting processes was not accurately modeled [22]. In the aforementioned studies, the experimentally measured relative humidity of concrete was chosen as the variable used to describe the variation in moisture content in concrete. Based on experimental results in the literature [23–26], a water vapor saturation phase exists at the early age of concrete, during which the relative humidity in the concrete remains at 100% following the development of hydration. Zhang et al. [26] proposed a subsection function to describe the water vapor saturation phase, but the modified function could not calculate the water content in different phases and may suffer from difficulty in the calibration of a considerable number of parameters.

Previous study of this work proposed and verified a modified hydration model of cement that has a clear distinction from other models in the existing literature [27]. Based on the modified hydration model and thermo-chemical coupled analysis, this paper examines the influence of water changes in concrete on the hydration process and investigates the hygro-thermo-chemical behaviors in concrete on a macroscale by adopting a homogenization scheme. In order to advance research work on the basis of previous studies, the moisture transport model is improved in this paper to describe the existence of the water vapor saturation stage in the early stage of the hydration reaction while retaining the original function. In addition, considering the different mechanisms of water transfer in different condition, the diffusion coefficients in dry and wet conditions are discussed and distinguished. The hygro-thermo-chemical parameters of the cement samples are obtained using a homogenization scheme. Numerical implementation is successfully achieved, and the simulation results of temperature and relative humidity are also compared with the experimental data.

2. Hygro-thermo-chemical model

2.1. A fixed model for the hydration process

The exothermic reaction of concrete occurs when water is combined with cement paste. To describe the degree of the reaction, the hydration extent is defined as the number of moles of water per unit volume. For practical purposes, it is convenient to rewrite the model in terms of a normalized variable, called a hydration degree, which is defined as

$$\xi(t) = \frac{w_n}{w_n\infty} \tag{1}$$

where $w_n\infty$ is the final mass of bound water under ideal conditions, assuming that the free water in the cement hydration process is completely reacted, and w_n is the mass of bound water formed by the hydration reaction at time t. ξ_∞ is the final hydration degree value under practical conditions. At the start of the hydration reaction, $\xi(t=0)=0$, and this value gradually increases with the progression of the chemical reaction.

According to Arrhenius's law, the time-dependent hydration progress can be described as shown in Eq. (2). In the model, the hydration rate is related to the temperature and the chemical affinity $A_\xi(\xi)$:

$$\frac{\partial\xi}{\partial t} = A_\xi(\xi)\exp\left(-\frac{E_a}{RT}\right) \tag{2}$$

where E_a is the activation energy of the reaction and R is the universal gas constant. Cervera et al. developed an analytical form of the normalized affinity based on thermodynamics [4]. The free energy of the thermo-chemical system can be divided into three parts: thermal contribution, thermo-chemical coupled contribution, and chemical contribution. The chemical contribution in this work is considered to be a quartic function instead of a cubic function. Similar to the strategy presented in the literature [4], a fixed form of the chemical affinity can be derived as follows:

$$A_\xi(\xi) = \beta_1(\beta_2+\beta_3\xi+\xi^2)(\xi_\infty-\xi)\exp\left(-\bar{\eta}\frac{\xi}{\xi_\infty}\right) \tag{3}$$

where β_1, β_2 and β_3 are material coefficients, ξ_∞ is the ultimate hydration degree and $\bar{\eta}$ represents the viscosity due to microdiffusion of the free water through the already formed hydrates. These parameters can be calibrated using experimental results.

In addition, it is generally known from experiments that the hydration process slows and may even stop with decreasing relative humidity. The effect of relative humidity on the hydration rate can be considered by improving Eq. (2) as follows:

$$\frac{\partial\xi}{\partial t} = \beta_h(h)A_\xi(\xi)\exp\left(-\frac{E_a}{RT}\right) \tag{4}$$

$$\beta_h(h) = \frac{1}{1+(a-ah)^4} \tag{5}$$

where $\beta_h(h)$ is an empirical function that was first proposed by Bažant [13], h is the relative humidity and a is a material parameter ranging from 5.5–12.5 that can be calibrated through the analysis of experimental data [18,20,21,28].

2.2. The transient heat transfer process

The transient heat transfer process of concrete can be described as follows:

$$\rho C\frac{\partial T(x,t)}{\partial t} = \lambda_T\Delta T(x,t) + \frac{\partial Q}{\partial t} \tag{6}$$

$$\frac{\partial Q}{\partial t} = Q_\infty\frac{\partial\xi}{\partial t} \tag{7}$$

where ρ, C, λ_T, Δ and Q_∞ are the density, volumetric heat capacity, thermal conductivity coefficient, Laplacian operator and final volumetric heat of hydration, respectively. The latent heat release due to concrete hydration is actually a nonlinear and thermally dependent process.

2.2.1. Heat capacity

Given the heat capacity values and volume fractions of cement, water and fine aggregates, the heat capacity of the matrix can be estimated using the law of mixtures [29]: