



A coupled hygro-thermal model of early-age concrete based on micro-pore structure evolution



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HIGHLIGHTS

- Coupling hygro-thermal model considers micro-pore structure evolution of early-age concrete.
- An innovative coefficient for counting the influence of humidity on hydration rate.
- Adsorption curve based on micro-pore structure evolution.
- Test verification procedures under different ambient temperature and humidity.

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ABSTRACT

In order to analyze the hygro-thermal coupling effect in early-age concrete, this research establishes a coupling hygro-thermal model based on hybrid mixture theory (HMT) considering the characteristic of the microstructure evolution of early-age concrete. The adsorption curve of early-age concrete is acquired based on the microstructure evolution through establishing the relationship between saturation and several factors, such as hydration degree, temperature, capillary pressure and so on. An innovative coefficient for counting the influence of humidity on hydration rate is proposed, which takes the influence of humidity on hydration rate under self-desiccation as a reference based on the existing test. The research results indicate that the coupled hygro-thermal model constructed based on the micro-pore structure evolution can accurately predict the time-dependent development of temperature and humidity field inside the early-age concrete. The research can theoretically support the investigation on the deformation and cracking of the early-age concrete.

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1. Introduction

With the proceeding of hydration in the early-age concrete, the heat releases and the water consumes because of the physical and chemical reactions. Meanwhile the chemical composition and pore structure of cementitious material change, which influences the diffusion properties of concrete, but also have a major impact on the mechanical properties of concrete. Large changes in temperature and humidity of early-age concrete will cause additional load, and even cause cracking of concrete, which will also affect the development of late strength of concrete and resistance to aggressive ions. Therefore the hygro-thermal coupling analysis in early-age concrete can be of great significance on the study of mechanical properties and corrosion resistance of the concrete structure. And it is the basis research of durability of concrete structures.

Numerous studies of the single temperature field or humidity field of early-age concrete can be found [1,2]. But the hygro-thermal diffusion properties in early-age concrete have obvious coupling effects [3–7]. While in the past research of hygro-thermal coupling, many scholars use heat and mass transfer model based on classical phenomenological theory [3,6], which mainly determines the model parameters on testing, and ignores important chemical reactions and pore structure changes in the early-age concrete. Heat and mass transfer model of porous media recently developed provides a good point of view for hygro-thermal coupling research. Ulm et al. [4] and Cervera et al. [5] established a thermo-chemo-mechanical model of early-age concrete based on thermodynamic theory in porous media, but did not consider the effect of humidity on the temperature and mechanical properties of concrete. Gawin et al. [7] had developed a more sophisticated early age concrete hygro-thermo-chemo-mechanical model based on hybrid mixture theory (HMT). In the model two separate diffusion equations were used

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to model separately the transport of water vapor and capillary water. But it did not take into account the pore characteristics (pore size, connectivity, etc.), which influences significantly diffusion properties of concrete.

In present work, a model describing hygro-thermal coupling phenomenon of early-age concrete considering the micro-pore structure evolution is proposed based on the works of Gawin et al. [7]. It is assumed that relative humidity (RH) is directly affected by the pore size of the concrete. And the relationship between saturation degree and several factors (such as hydration degree, temperature, and relative humidity) is re-established. The effect of pore relative humidity on the rate of hydration is comprehensively analyzed, which takes the change of relative humidity in the case of the self-desiccation as a reference.

2. General conservation equations

The model consists of a fully coupled hygro-thermal formulation where concrete is treated as a multiphase system consisting of solid, liquid and gas phases. The pore of solid skeleton is filled by liquid and gas phase. The liquid phase is considered to include adsorbed water (physically bound to the surface of the solid skeleton) and capillary water. The gas phase is considered to be a mixture of dry air and water vapor, both of which are assumed to behave as ideal gases. The model equations are obtained by means of the hybrid mixture theory (HMT) proposed by Hassanizadeh and Gray [8–10]. For sake of brevity only the most essential aspects, the simplifications of the mathematical formulation are given here. To simplify the general reference formulation [7] the following assumptions are introduced:

- (i) There is thermal equilibrium balance between all phases within an infinitesimal volume.
- (ii) The velocity of the solid skeleton is negligible compared to those of the fluid phases.
- (iii) The bound water does not flow. It flows and evaporates only after it is released as free water.

Starting from the micro-scale thermodynamic equilibrium and assuming (i)–(iii), the macroscopic balance equations are obtained for dry air (1), water (Inc. liquid water and water vapor) (2), and enthalpy (3).

$$\frac{\partial(\varepsilon_G \rho_A)}{\partial t} - \nabla \cdot \left[\varepsilon_G \rho_G \frac{M_A M_V}{M_G^2} \mathbf{D}_G \nabla \left(\frac{P_A}{P_G} \right) \right] - \nabla \cdot \left(\varepsilon_G \rho_A \frac{\mathbf{K} \mathbf{K}_G}{\mu_G} (\nabla P_G - \varepsilon_G \rho_G \mathbf{g}) \right) = 0 \quad (1)$$

$$\frac{\partial(\varepsilon_G \rho_V)}{\partial t} + \frac{\partial(\varepsilon_L \rho_L)}{\partial t} - \nabla \cdot \left[\varepsilon_L \rho_L \frac{\mathbf{K} \mathbf{K}_L}{\mu_L} \nabla (P_G - P_C - \varepsilon_L \rho_L \mathbf{g}) \right] - \nabla \cdot \left[\varepsilon_G \rho_G \frac{M_A M_V}{M_G^2} \mathbf{D}_G \nabla \left(\frac{P_V}{P_G} \right) \right] - \nabla \cdot \left[\varepsilon_G \rho_V \frac{\mathbf{K} \mathbf{K}_G}{\mu_G} (\nabla P_G - \varepsilon_G \rho_G \mathbf{g}) \right] = -\dot{M}_h \quad (2)$$

$$(\rho C)_{\text{eff}} \frac{\partial T}{\partial t} - \nabla \cdot (\lambda \nabla T) - [\varepsilon_L \rho_L C_L \frac{\mathbf{K} \mathbf{K}_L}{\mu_L} \nabla (P_G - P_C - \varepsilon_L \rho_L \mathbf{g}) \cdot \nabla T - \varepsilon_G \rho_G C_G \frac{\mathbf{K} \mathbf{K}_G}{\mu_G} (\nabla P_G - \varepsilon_G \rho_G \mathbf{g}) \cdot \nabla T] = -\dot{M}_{va} \Delta H_v + \dot{M}_h \Delta H_h \quad (3)$$

where symbols S, L, G, A and V denote solid skeleton, liquid water, gas phase, dry air and vapor, respectively. P_C is the capillary pressure ($P_C = P_G - P_L$), ε_π is the volume fraction of a phase π , ρ_π is the

density of a phase π , M_A , M_V and M_G are the molar masses of dry air, water vapor and gas respectively, \mathbf{K} is the intrinsic permeability tensor, K_π and μ_π are the relative permeability and the dynamic viscosity of the phase π , \mathbf{D}_G is the effective diffusivity tensor for the dry air/water vapor mixture within the porous concrete, M_h means mass of hydrated water, M_{va} is the mass of vaporized water, ΔH_v is the specific enthalpy of evaporation, ΔH_h is the latent heat of hydration, T is the absolute temperature. $(\rho C)_{\text{eff}}$ is the effective heat capacity of concrete: $(\rho C)_{\text{eff}} = \rho_s C_s + \rho_L C_L + \rho_G C_G$, where C_π is the specific isobaric massive heat of the phase π . The porosity is denoted by ϕ ($\phi = \varepsilon_G + \varepsilon_L$), S is the saturation degree of the liquid phase ($S = \varepsilon_L / \phi$).

3. The hydration model

Hydration of cement is a complex physical and chemical reaction process. The various components of the cement particles react with water and the gel is produced, so that the concrete has strength and stiffness. Although many scholars have studied the hydration mechanism, but we still cannot accurately calculate the chemical reaction process. The impact of external factors (temperature, humidity, etc.) on the chemical reaction is still in research. Therefore, most scholars [4,11] considered the cement hydration as an overall hydration process rather than the chemical reactions of individual components.

Several hydration models based on micro-structure evolution have been proposed previously (DUCOM [12], HYMOSTRUC [13], etc.). These models are usually used to describe the change of cement particle during hardening with great realism, but are not really appropriate for applications in finite element computation. Ulm and Coussy [4] considered the water diffusion process through the layer of hydrated compounds as the dominant mechanisms governing the hydration kinetics. And the model was later revisited by Cervera et al. [5]. The hydration process can be described by means of a normalized measure called hydration degree, which is defined as

$$\alpha = \chi / \bar{\chi}_\infty \quad (4)$$

where χ is the hydration extent, $\bar{\chi}_\infty$ is the final values of hydration extent in ideal hygrometric conditions. The actual final value of hydration extent, χ_∞ , is always smaller than the theoretical value. The ratio between the actual and the theoretical final values is the final values of hydration degree $\alpha_\infty = \chi_\infty / \bar{\chi}_\infty$. Cervera et al. [5] proposed the following evolution equation for the hydration degree

$$\dot{\alpha} = A(\alpha) \beta(H) \exp \left(-\frac{E_a}{RT} \right) \quad (5)$$

and

$$A(\alpha) = A_1 \left(\frac{A_2}{\alpha_\infty} + \alpha \right) (\alpha_\infty - \alpha) \exp \left(-\eta \frac{\alpha}{\alpha_\infty} \right) \quad (6)$$

where $A(\alpha)$ is the normalized chemical affinity, E_a is the hydration activation energy, R is the universal gas constant, and A_1 , A_2 and η are material parameters. H is the relative humidity, $\beta(H)$ is the effect of relative humidity on the hydration rate, which is an empirical function that was proposed for the definition of the equivalent hydration period [7,14]. But recently, some studies [15,16] think that the decrease of relative humidity is the intrinsic characteristics of hydration reaction in self-desiccation condition, which has been reflected in the chemical affinity. Consequently, it is not necessary to consider the influence in this situation.

Contrarily to self-desiccation, when the moisture migrates in concrete, i.e. when moisture increased or reduced with respect to the moisture in self-desiccation condition, the influence of relative humidity on the hydration process should be considered. Gerstig

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