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Properties prediction of ultra high performance concrete using blended cement hydration model

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HIGHLIGHTS

- Proposed a hydration model of ultra high performance concrete (UHPC).
- Considered both cement hydration and silica fume reaction.
- Predicted degree hydration of cement, CH contents and mechanical properties.
- Proposed model is valid for both ordinary strength concrete and UHPC.

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ABSTRACT

Ultra high performance concrete (UHPC) consists of cement, silica fume (SF), sand, fibers, water and superplasticizer. Typical water/binder-ratios are 0.15–0.20 with 20–30% of silica fume. The development of properties of hardening UHPC relates with both hydration of cement and pozzolanic reaction of silica fume. In this paper, by considering the production of calcium hydroxide in cement hydration and its consumption in the pozzolanic reaction, a numerical model is proposed to simulate the hydration of UHPC. The degree of hydration of cement and degree of reaction of silica fume are obtained as accompanied results from the proposed hydration model. The properties of hardening UHPC, such as degree of hydration of cement, calcium hydroxide contents, and compressive strength, are predicted from the contribution of cement hydration and pozzolanic reaction. The proposed model is verified through experimental data on concrete with different water-to-binder ratios and silica fume substitution ratios.

1. Introduction

Concrete or cementitious composites with compressive strength over 150 MPa are generally described as ultra-high performance concrete (UHPC); if fibers are added in order to decrease brittleness and increase energy absorption capacity the term ultra-high performance fiber reinforced concrete (UHP-FRC) is used. UHPC's high compressive strength, obtained through dense particle packing, implies high durability, improved resistance against freeze–thaw cycles and various chemicals as well as higher penetration resistance [1,2].

Many experimental studies have been done on the development of properties and proportioning mixtures of UHPC. Morin et al. [3] found that for reactive powder concrete (RPC), a long dormant period of about 30 h after water addition which was attributed to the high amount of superplasticizer. Then, the hydration started and was characterized by a strong heat release, which lasted for about 12 h. Bentz et al. [4] and Chung [5] reported that silica fume (SF) fulfils some functions in UHPC: it fills voids between cement grains, it enhances the rheological characteristics and it forms hydration products by pozzolanic activity. Another important effect of the silica fume is the improvement of the interfacial transition zones between binder and steel fibers. Thus, the mechanical strengths are increased and microstructure and packing efficiency of the UHPC are enhanced. Loukili et al. [6] investigated the hydration kinetics, change of relative humidity, and autogenous shrinkage of ultra-high-strength concrete. They found that the degree of hydration of cement is only 0.58 at 28 days due to the lower water to binder ratio in ultra high strength concrete, and the autogeneous shrinkage of ultra high strength concrete were much higher than ordinary strength concrete because of high self-desiccation at an early age due to both a very low w/c ratio and a high silica fume content.

Besides experimental investigations on chemical and physical properties of UHPC [3–6], there are some theoretical models for

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Nomenclature

α	degree of cement hydration
v	stoichiometric ratio by mass of water to cement
w_g	physically bound water in C–S–H gel
ρ_w	density of water
S	Blaine surface area
ρ_c	density of the cement
r_0	radius of unhydrated cement particles
S_w	effective surface area of the cement particles in contact with water
S_0	total surface area if the surface area develops unconstrained
B	the parameter controls the rate of the initial shell formation
C	the parameter controls the rate of the initial shell decay
k_d	cement hydration rate coefficient in the initial dormant period
k_r	cement hydration rate coefficient in the phase boundary reaction period
D_e	effective diffusion coefficient of water in cement hydration products
D_{e0}	initial value of D_e
B_{20}, C_{20}, k_{r20}, and D_{e20}	values of B, C, k_r, and D_{e0} at 20 °C, respectively
β_1, β_2, E/R, and β_3	temperature sensitivity coefficients of B, C, k_r, and D_{e0}, respectively
C_0	mass of cement in the mix proportion
W_0	mass of water in the mix proportion
$C_{w\text{-}free}$	amount of water at the exterior of the C–S–H gel
r	empirical parameter considering the accessibility of water into an inner anhydrous part
$CHCE(t)$	mass of produced calcium hydroxide from the hydration of cement
SF	silica fume
CH	calcium hydroxide
α_{silica}	degree of reaction of the glass (active) phase of silica fume
$m_{silica0}$	silica fume mass in mixing proportion
γ_s	mass percentage of glass silica in silica fume
W_{cap} and W_{chem}	masses of capillary water and chemically bound water, respectively
$m_{CH}(t)$	mass of calcium hydroxide in hydrating cement–silica fume blends
v_{si}	stoichiometry ratio by mass of CH to silica fume
r_{si0}	radius of silica fume particle
D_{esi}	reaction rate coefficient of silica fume in the diffusion period
D_{esi0}	initial value of D_{esi}
k_{rsi}	reaction rate coefficient of silica fume during the phase boundary reaction period
D_{esi20} and k_{rsi20}	values of D_{esi0}, and k_{rsi} at 293 K, respectively
β_{esi} and E_{si}/R	temperature sensitivity coefficients of D_{esi0}, and k_{rsi}, respectively
φ	capillary porosity in hydrating silica fume–cement paste
α_{CEc} and α_{SFc}	critical reaction degrees of cement and silica fume corresponding to percolation threshold of capillary porosity, respectively
x_{fc}	gel/space ratio of blended cement pastes
f_c	compressive strength of blended concrete
A	intrinsic strength of cement and silica fume blends
a and b	contributions of cement and silica fume to the intrinsic strength, respectively
n	strength exponent
c and d	contributions of cement and silica fume to the strength exponent, respectively

predicting properties of silica fume blended concrete or UHPC. Based on a simplified scheme describing the activity of silica fume and fly ash in terms of chemical reactions, Papadakis [7] evaluated the final chemical and volumetric composition of supplementary cementing materials (SCM) concrete. Furthermore, carbonation of the SCM concrete was predicted. Ishida et al. [8] proposed a model to predict the micro–hygro–physical properties of high strength blended concrete and ordinary strength concrete. Mechanical properties, water desorption, moisture loss and drying shrinkage behaviors were determined by an enhanced intrinsic porosity model. Zelic et al. [9] developed a mathematical model to predict the development of compressive strength in cement–silica fume blends. Knudsen's dispersion models were applied in fitting both the degree of hydration and the compressive strength experimental data as a function of time. It was found that the degree of hydration—the compressive strength dependence, for replacement levels varying from 0% to 15% mass of silica fume, indicates a linear mathematical function. Using semi-adiabatic heat of hydration tests, Habel et al. [10] proposed a kinetic hydration model for ultra high performance concrete, and evaluated mechanical properties of hardening UHPC. Compressive strength, tensile strength, fracture energy and secant modulus were evaluated from degree of reaction. It was observed that for the UHPC, the rate of development of mechanical properties was highest for the secant modulus, followed by the compressive and then the tensile strength.

As shown in Refs. [8–10], the development of properties of silica fume blended concrete or UHPC relates with degree of hydration. On the other hand, Papadakis [7] proposed that the development of properties of silica fume blended concrete relates with both cement hydration and silica fume pozzolanic reaction. In this paper, a numerical model is proposed to simulate the hydration of UHPC. The degree of hydration of cement and degree of reaction of silica fume are obtained as accompanied results from the proposed hydration model. The properties of hardening UHPC are predicted from the contribution of cement hydration and pozzolanic reaction.

2. Hydration model of Portland cement

The shrinking-core model, which was originally developed by Tomosawa [11], is used in this study to simulate the development of cement hydration. This model is expressed as a single equation consisting of three coefficients: k_d the reaction coefficient in the induction period; D_e the effective diffusion coefficient of water through the C–S–H gel; and k_r a coefficient of the reaction rate of cement as shown in Eq. (1). These coefficients determine the rate of mass transport through the initial shell layer, the rate of phase boundary reaction process, and the rate of diffusion controlled process. The modeled cement particles are assumed to be spheres surrounded by hydration product. Based on this theory, the rate of cement hydration is derived as follows:

$$\frac{d\alpha}{dt} = \frac{3(S_w/S_0)\rho_w C_{w\text{-}free}}{(v+w_g)r_0\rho_c} \frac{1}{\left(\frac{1}{k_d}-\frac{r_0}{D_e}\right)+\frac{r_0}{D_e}(1-\alpha)^{\frac{-1}{3}}+\frac{1}{k_r}(1-\alpha)^{\frac{-2}{3}}} \quad (1)$$

where α is the degree of cement hydration; v is the stoichiometric ratio by mass of water to cement (= 0.25); w_g is the physically bound water in C–S–H gel (= 0.15); ρ_w is the density of water;