Construction and Building Materials 54 (2014) 197–201

Contents lists available at ScienceDirect

Construction and Building Materials

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

A numerical method for predicting Young's modulus of heated cement paste

Jie Zhao [a,*], Jian-Jun Zheng [b], Gai-Fei Peng [a]

[a] *School of Civil Engineering, Beijing Jiaotong University, Beijing 100044, PR China*
[b] *School of Civil Engineering and Architecture, Zhejiang University of Technology, Hangzhou 310014, PR China*

HIGHLIGHTS

- A numerical method is developed for predicting the Young's modulus of heated cement paste.
- Thermal decomposition analysis of cement paste is conducted.
- The effects of thermal decomposition and microcracking on the Young's modulus of heated cement paste are considered.

ARTICLE INFO

Article history:
Received 2 August 2013
Received in revised form 10 December 2013
Accepted 17 December 2013
Available online 14 January 2014

Keywords:
Cement paste
Young's modulus
High temperature
Thermal decomposition
Microcracking

ABSTRACT

The evaluation of the mechanical properties of heated cement paste is essential to the safety assessment of concrete structures exposed to elevated temperatures. A numerical method is developed in this paper for predicting the Young's modulus of heated cement paste with or without silica fume up to 600 °C. The initial volume fractions of various constituents and the thermal decomposition of hydration products in cement paste are approximately estimated. A two-phase composite sphere model is then built and a two-step approach is applied to evaluating the Young's modulus of heated cement paste with thermal decomposition and microcracking effects. Finally, the validity of the proposed numerical method is verified with three sets of experimental data collected from the literature.

1. Introduction

Young's modulus of heated cement paste is essential to the stiffness evaluation of concrete structures under high temperature conditions and therefore has been studied experimentally and theoretically. Dias et al. [1] showed that the mechanical properties of heated cement paste are characterized by the highest temperature ever experienced by the material. At the temperatures of 300 and 600 °C, two remarkable drops in Young's modulus were observed. Using the non-destructive ultrasonic technique, Masse et al. [2] found a decreasing trend of the Young's modulus of cement pastes at different curing ages with the heating temperature. Odelson et al. [3] and Kerr [4] observed that the stiffness loss of heated cement paste occurs predominantly below 120 °C and concluded that the loss is mainly attributed to microcraking. Padevět and Zobal [5] found a drastic decrease in Young's modulus of cement paste at a heating temperature of 450 °C. Compared with experimental investigations, theoretical analyses are relatively few. Ulm et al. [6] analyzed the Channel Tunnel fire using a linear relationship between the dehydration degree and Young's modulus of concrete. In Lee et al.'s model [7], the decomposition degree of various constituents in cement paste was taken as a linear function of temperature and the Young's modulus of heated cement paste was estimated by applying the theory of composite damage mechanics. However, microcracking of cement paste is not considered explicitly. All of the aforementioned research clearly shows that it is still highly desirable that a numerical method can be available for evaluating the Young's modulus of heated cement paste with thermal decomposition and microcracking effects.

The purpose of this paper is to predict the Young's modulus of heated cement paste with or without silica fume up to 600 °C. After the initial volume fractions of various constituents in cement paste are formulated in an approximate manner, the thermal decomposition of cement paste is analyzed. By applying a two-phase composite sphere model and a two-step procedure, the effects of thermal decomposition and microcracking on the Young's modulus of heated cement paste are modeled. Finally, the validity of the proposed method is verified with three sets of experimental data.

---

* Corresponding author. Tel.: +86 10 51684866.
E-mail address: zhaojie@bjtu.edu.cn (J. Zhao).

0950-0618/$ - see front matter © 2013 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.conbuildmat.2013.12.070

2. Initial volume fractions of various constituents in cement paste

To predict the thermal decomposition, the initial volume fractions of various constituents in cement paste have to be estimated. Usually, they can be expressed as a function of the water to binder ratio, the degree of hydration, and the chemical composition of cement. When silica fume is added, the pozzolanic reaction needs to be taken into account.

It has been shown that, at complete hydration, the volume of cement gel generated from 1 g of cement is 0.682 cm^3 [8]. By taking the specific gravity of Portland cement as 3.15, the volume fractions of unhydrated cement and cement gel in hardened cement paste are given by

$$f_{unhyC} = \frac{0.32(1-\alpha_c)}{w/c+0.32} \tag{1}$$

$$f_{gel} = \frac{0.68\alpha_c}{w/c+0.32} \tag{2}$$

where α_c is the degree of hydration of cement and w/c is the water to cement ratio. If a mass fraction S of cement is replaced with silica fume and its degree of hydration is taken as zero, f_{unhyC} and f_{gel} are modified as

$$f_{unhyC} = \frac{0.32(1-\alpha_c)(1-S)}{w/c+0.32(1-S)+S/\rho_{SF}} \tag{3}$$

$$f_{gel} = \frac{0.68\alpha_c(1-S)}{w/c+0.32(1-S)+S/\rho_{SF}} \tag{4}$$

where ρ_{SF} is the density of silica fume and w/c is converted into the water to binder ratio.

According to Bentz and Garboczi [9], each volume unit of C_3S produces 1.7 volume units of C–S–H and 0.61 volume units of CH; each volume unit of C_2S produces 2.39 volume units of C–S–H and 0.191 volume units of CH; and each volume unit of C_3A produces 1.69 volume units of hydrated aluminates. It is assumed in this paper that each unit volume of C_4AF produces the same amount of hydration products as C_3A. With these parameters, the volume fractions of CH (f_{gel}^{CH}), hydrated aluminates (f_{gel}^{AL}), and C–S–H (f_{gel}^{CSH}) in hydration products can be evaluated.

For silica fume, which consists primarily of amorphous silicon dioxide, a k-value of 1.0 is usually applied. The pozzolanic reaction of silica fume can be expressed as [10]

$$\underset{1.35}{1.1\mathrm{CH}} + \underset{1}{\mathrm{S}} + \underset{1.87}{2.8\mathrm{H}} \rightarrow \underset{3.77}{\mathrm{C}_{1.1}\mathrm{SH}_{3.9}} \tag{5}$$

where the number below each reactant represents the volume stoichiometry. Thus, the initial volume fractions of pozzolanic C–S–H (f_{pCSH}^0), CH (f_{CH}^0), conventional C–S–H (f_{CSH}^0), and hydrated aluminates (f_{AL}^0) can be respectively estimated for a given degree of hydration of silica fume α_s as follows

$$f_{pCSH}^0 = \frac{3.77S\alpha_s/\rho_{SF}}{w/c+0.32(1-S)+S/\rho_{SF}} \tag{6}$$

$$f_{CH}^0 = f_{gel}\cdot f_{gel}^{CH} - \frac{1.35S\alpha_s/\rho_{SF}}{w/c+0.32(1-S)+S/\rho_{SF}} \tag{7}$$

$$f_{CSH}^0 = f_{gel}\cdot f_{gel}^{CSH} \tag{8}$$

$$f_{AL}^0 = f_{gel}\cdot f_{gel}^{AL} \tag{9}$$

It should be mentioned that Eqs. (1)–(9) are only valid for traditional cement paste or silica fume blended cement paste. If fly ash or other types of supplementary cementitious materials are added, a new set of expressions needs to be established.

3. Thermal decomposition analysis of cement paste

With the decomposition prediction method proposed by Zhao et al. [11], the conversion degree of each constituent in cement paste can be determined. Thus, the volume fractions of decomposed constituents f_i^d are equal to

$$f_i^d = f_i^0 a_i \tag{10}$$

where a_i and f_i^0 are the conversion degree and initial volume fraction of reactant i (i = CH, AL, and C–S–H), respectively. The water decomposed from the reactants is regarded as additional pores and the volume fraction f_i^w is given by

$$f_i^w = f_i^d n_i^w \frac{\rho_i/M_i}{\rho_w/M_w} \tag{11}$$

where n_i^w is the amount of water in mole decomposed per mole of reactant i, ρ_w and M_w are the density and molar mass of water, and ρ_i and M_i are the density and molar mass of reactant i, respectively.

It was showed from a detailed analysis [11] that, $n_{CH}^w = 1.0$, $\rho_{CH} = 2.24\,\mathrm{g/cm^3}$, and $M_{CH} = 74$ g/mol for CH; $n_{Al}^w = 20$, $\rho_{AL} = 1.8\,\mathrm{g/cm^3}$, and $M_{AL} = 1255$ g/mol for hydrated aluminates; and $n_{CSH}^w = n_{pCSH}^w = 3.0$, $\rho_{CSH} = \rho_{pCSH} = 1.75\,\mathrm{g/cm^3}$, and $M_{CSH} = M_{pCSH} = 365$ g/mol for conventional and pozzolanic C–S–H. The initial volume fractions of the solid phase in conventional and pozzolanic C–S–H are respectively equal to

$$f_{CSH}^s = (1 - f_{CSH}^{gelp})f_{CSH}^0 \tag{12}$$

$$f_{pCSH}^s = (1 - 0.19)f_{pCSH}^0 \tag{13}$$

where f_{CSH}^{gelp} is the volume fraction of gel pores in conventional C–S–H and given by

$$f_{CSH}^{gelp} = 0.28/f_{gel}^{CSH} \tag{14}$$

Thus, the total initial volume fraction of the solid phase in C–S–H is

$$f_{CSH}^{0s} = f_{CSH}^s + f_{pCSH}^s \tag{15}$$

Substitution of Eq. (15) into Eq. (11) yields the volume fraction of water released from the decomposition of C–S–H. Division of the volume fraction of water released from each reactant by the volume fraction of the converted reactant yields the porosities of decomposition products of hydrated aluminates (f_{AL}^{pp}), CH (f_{CH}^{pp}), conventional C–S–H (f_{CSH}^{pp}), and pozzolanic C–S–H (f_{pCSH}^{pp})

$$f_{AL}^{pp} = n_{AL}^w \frac{\rho_{AL}/M_{AL}}{\rho_w/M_w} = 0.52 \tag{16a}$$

$$f_{CH}^{pp} = n_{CH}^w \frac{\rho_{CH}/M_{CH}}{\rho_w/M_w} = 0.54 \tag{16b}$$

$$f_{CSH}^{pp} = n_{CSH}^w \frac{\rho_{CSH}/M_{CSH}}{\rho_w/M_w} + \frac{0.28}{f_{gel}^{CSH}} = 0.58 \tag{16c}$$

$$f_{pCSH}^{pp} = n_{CSH}^w \frac{\rho_{CSH}/M_{CSH}}{\rho_w/M_w} + 0.19 = 0.40 \tag{16d}$$

It should be mentioned that, since the volume fraction of C–S–H in gel is around 0.65 for most commonly used cement, f_{gel}^{CSH} is taken as 0.65 in Eq. (16c).

4. Young's modulus of heated cement paste

In predicting the Young's modulus of heated cement paste, two main factors are considered: one is the thermal decomposition of hydration products and the other is cracks formed in the cement