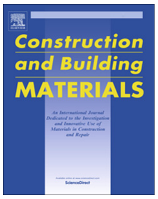
Construction and Building Materials 172 (2018) 330–339

Contents lists available at ScienceDirect

Construction and Building Materials

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



Analytical and numerical modeling of elastic moduli for cement based composites with solid mass fractal model

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HIGHLIGHTS

- The solid mass fractal model describes well pore-solid structure in cement paste.
- Analytical modeling of elastic moduli is performed using effective medium theory.
- Numerical modeling of elastic moduli is performed using finite element method.

ARTICLE INFO

Article history:
Received 4 December 2017
Received in revised form 23 March 2018
Accepted 29 March 2018

Keywords:
Cement based composites
Elastic moduli
Solid mass fractal model
Effective medium theory
Finite element method

ABSTRACT

Elastic moduli are of the critical parameters in performance design and analysis for cement based composites. As a result of the intrinsic heterogeneity, however, the prediction of elastic moduli remains a practical challenge. In this paper, the solid mass fractal model is applied, which builds up the pore-solid structure of slag-blended cement paste in conjunction with the mercury intrusion porosimetry test. Moreover, the analytical and the numerical modeling of elastic moduli are performed making use of the effective medium theory and the finite element method, respectively. For the sake of validation, the elastic moduli from modeling are compared with those measured from the ultrasonic wave test. Most of all, this paper intends to propose a novel method that predicts well the elastic moduli of cement based composites.

1. Introduction

Elastic moduli such as the Young's modulus, the bulk modulus and the shear modulus are of the critical parameters in performance design and analysis for cement based composites [1]. Due to the paramount importance, a number of modeling methods have been proposed so far which might be analytical or numerical [2–6]. Generally, the analytical methods refer to establishing some specific micromechanical models, which aim at predicting elastic moduli of cement based composites from the knowledge of their geometric and physical characteristics [2–4]. In comparison, the numerical methods are fairly straightforward, which primarily rely on heavy computations to solve basic equations of stiffness [5,6]. As a matter of fact, being the intrinsic porous medium for cement based composites, the accuracy of modeling predominantly depends on characterization of the associated pore-solid structure.

It is well known that the pore-solid structure in cement based composites manifests an extreme heterogeneity over several orders from nanometers (nm) to micrometers (μm) [7]. At the nanoscale, basic globules of around 5 nm are packed to form the porous calcium silicate hydrate (C-S-H) gel; at the microscale, unreacted species and hydration products are agglomerated in a random manner [8–11]. Therefore, a fundamental modeling of pore-solid structure as well as various properties including elastic moduli necessitates addressing the multiscale issue for cement based composites. For instance, Bernard et al. proposed a two-level homogenization method for Portland cement paste, where the Mori-Tanaka method and self-consistent scheme were applied in the nanoscale C-S-H gel and microscale cement paste, respectively [12]. Note that as it has to assign a large number of parameters and assumptions in bridging the nanoscale and microscale pore-solid structure, the multiscale approach often leads to a substantial disadvantage in efficiency and operability, which shall be even more pronounced for blended cementitious systems [13,14].

During past decades, the fractal character has been well recognized for the pore-solid structure in cement based composites [15–19]. It was argued that three types of fractal might be present, i.e., the pore mass fractal, the pore surface fractal and the solid mass fractal. In essence, the fractal character is to describe a complex

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https://doi.org/10.1016/j.conbuildmat.2018.03.267
0950-0618/© 2018 Published by Elsevier Ltd.

Nomenclature

P	intrusion pressure
γ_s	surface tension of mercury
L	linear length of Euclidean space in solid mass fractal model
N	number of subregions for solid mass fractal model
w	proportion of iterating phase in generator of solid mass fractal model
i	number of iteration step for solid mass fractal model
χ, χ_i	solid fraction or relative density
D	solid mass fractal dimension
K_0, G_0	bulk and shear moduli of basic element
υ_0	Poisson's ratio of basic element
k,g	dimensionless coefficients
c	volume fraction of embedded particles
Θ	elastic energy
α, β	labels running over the components of strain
$C_{\alpha\beta}$	elastic modulus tensor of the pixel
p,q	labels running over the 3 directions
M	shape function for a cubic tri-linear finite element
T	conversion operator imposed on the shape function
C_w	wave speed in ultrasonic wave test
υ	Poisson's ratio
d	equivalent pore diameter
θ	contact angle of imperfect wetting
n	number of subregions in each dimension for solid mass fractal model
b	number of iterating phase in generator of solid mass fractal model
d_i	size of element after i steps for solid mass fractal model
V_{tot}, V	total volume, pore volume
f	cumulative porosity
d_{upp}, d_{low}	lower and upper limits of pore diameter
E_0	Young's modulus of basic element
K_i, G_i	bulk and shear moduli of inclusion phase
K_m, G_m	bulk and shear moduli of matrix
x, y, z	Cartesian coordinates
ε_α,ε_β	local strains at a point (x, y, z) within the pixel
r,s	labels running over the 8 nodes
u	nodal displacement
S	conversion function from displacement to strain
Ψ	stiffness matrix for a pixel
ρ	apparent density
E	Young's modulus
K, G	bulk and shear moduli

phenomenon or object that exhibits the similar pattern at different scales, i.e., the so-called self-similarity. If one-dimensional length of fractal is magnified, the occupied area or space of fractal is also magnified which follows a power law. Making use of the fractal character, the nanoscale and microscale pore-solid structure of cement based composites could be well bridged in terms of the self-similarity, which shall lead to much reduced cost compared with the conventional multiscale approach [20].

In a previous study, upon a comprehensive examination on the fractal character of pore-solid structure in cement based composites, it was revealed that the solid mass fractal could be the most probable type [21]. Moreover, a fractal based structural model, i.e., the solid mass fractal model was developed [22]. In this paper, the solid mass fractal model and the mercury intrusion porosimetry (MIP) test are to model the pore-solid structure of a blended cementitious system, i.e., Portland cement blended with blast furnace slag. Then, the analytical and the numerical modeling of elastic moduli are performed making use of the effective medium theory and the finite element method, respectively. For the sake of validation, results of elastic moduli from modeling are compared with those from the ultrasonic wave test.

2. Materials

The slag-blended cement pastes were examined. Chemical compositions of Portland cement and blast furnace slag are listed in Table 1. The mix proportions are given in Table 2. In particular, three groups of paste specimens were prepared with the dosage of slag varying from 10%, 20% to 40%, as denoted by P10, P20 and P40. The water to binder (w/b) ratio was 0.4. The curing age was 28 days. Six prismatic specimens of 40 × 40×160 mm^3 were cast for each group, as shown in Fig. 1. Fresh pastes were firstly cured in the curing room (95 ± 10% relative humidity and 20 ± 1 °C temperature) for 24 h. Then, the demolded specimens were further cured until the designed age. Thereafter, three of the specimens in each group were broken to collect small pieces towards the MIP test on one hand. The other three specimens were kept integrated and subjected to the ultrasonic wave test on the other hand.

Table 1
Chemical composition of cement and slag (% by mass).

Binder	CaO	SiO_2	Al_2O_3	Fe_2O_3	SO_3	MgO	Others
Cement	66.93	21.67	5.05	3.73	2.62	–	–
Slag	37.12	32.72	15.51	0.28	2.61	5.50	6.26

3. Mercury intrusion porosimetry

The MIP test was adopted to characterize the pore size distribution of slag-blended cement paste [23,24]. Samples of the collected small pieces were immersed in liquid nitrogen for five minutes to prevent further hydration. Then, the low temperature vacuum freeze drying was carried out that might reduce possible microcracks during drying process. The sample mass was then monitored until it reached a stable loss of 0.01% per day. Such period of drying could last about two weeks. The dried sample was subjected to the MIP test. As shown in Fig. 2, the applied intrusion pressure in MIP test was increased from 0 to 206 MPa. In common, pores are idealized as cylindrical tubes with various diameters, and thus the intrusion pressure P can be related to the equivalent pore diameter d via the Laplace equation as follows,

$$P = \frac{4\gamma_s \cos\theta}{d} \tag{1}$$

where γ_s is the surface tension of mercury, and θ is the contact angle of imperfect wetting between mercury and pore surface. Herein, γ_s = 0.48 N/m and θ = 140° are applied [23]. The pore size distribution is presented in terms of the cumulative porosity versus the pore diameter, as shown in Fig. 3.

Table 2
Mix proportions of pastes.

Paste	Dosage of binder (% by mass)		w/b
	Cement	Slag	
P10	90	10	0.4
P20	80	20	
P40	60	40	