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Fractal and multifractal analysis on pore structure in cement paste

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HIGHLIGHTS

- We perform fractal and multifractal analysis on cement paste.
- The fractal dimension depends linearly on porosity.
- The multifractal spectrum accounts for more structural details.

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ABSTRACT

The capillary pore structure in cement paste is critical to the transport property, to which various durability problems of concrete are closely related. A novel characterization of pore structure in cement paste has to account for its intrinsic heterogeneity, i.e., the disordered porous media. In this paper, we present some results about the application of fractal and multifractal analysis on simulated pore structure of cement paste, where some hydration factors including the water to cement ratio and the degree of cement hydration are discussed in terms of the fractal dimension and the multifractal spectrum. Results indicate that the concepts of fractal and multifractal are feasible in characterizing the heterogeneity of pore structure in cement paste. Moreover, it is confirmed that compared to the fractal concept, the multifractal concept allows a relatively more reasonable characterization, where the size distribution and the spatial arrangement of pore are addressed without any priori assumptions.

1. Introduction

Pores are the inherent constituents in concrete. The size of various types of pores can range from nm to mm, i.e., from the calcium silicate hydrate gel pore to air voids. In practice, the capillary pore in cement paste with the size of μm is believed to be of critical importance to the transport property of concrete, to which various durability problems are closely related [1].

As known, the capillary pore structure in cement paste is of extreme heterogeneity. Hereafter, if not specified, the capillary pore is abbreviated as pore in this paper. On one side, the geometrical shape of pore is irregular, which cannot be described by a single mathematical formula analytically [2]. On the other side, the spatial arrangement of pore is disordered, where the concept of tortuosity for pore pathway has often to be discussed [3]. The intrinsic heterogeneity of pore structure makes the capturing of its characteristic a practical challenge. In general, the pore size distribution is defined to characterize the pore structure, i.e., the volume fraction of pore against a size grade. For instance, within a mercury intrusion porosimetry (MIP) test, the cumulative volume of intruded mercury is recorded against the applied pressure, and then the pore size distribution can be derived [4]. Nevertheless, it has to be noted that for a disordered porous media, the relevant performances can be affected by the spatial arrangement of pore as well, such as permeability [5,6]. Thus, a novel characterization of the pore structure has to account for both the pore size distribution and the pore spatial arrangement.

In a pioneering work, Winslow reported that the internal surface of cement paste was essentially fractal [7]. Thereafter, the fractal property of cement paste has drawn a lot of attention in past decades [8–14]. As examined by Lange et al., the pore structure in cement paste displayed a fractal behavior as well [8]. Within a fractal description, the pore spatial arrangement can be described by a self-similarity regardless of the measurement scale. Meanwhile, the pore size distribution can be addressed by the fractal dimension in terms of a power law relation [15]. Studies also indicate that the fractal dimension can be used to predict various

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Nomenclature

i	serial number for pixel
I	pixel value of 0 or 1
D	fractal dimension
N	number of boxes to cover the pore space
L	total length in one dimension
f	porosity
P	probability to find a box covering pore space
V^*	cumulative pore volume fraction
t	coefficient function
c	constant
n	number of grid boxes for the whole structure
m	number of pore pixels in a grid box
M	total number of pore pixels for the whole structure
$f(\alpha)$	multifractal spectrum
$N_\alpha(\delta)$	number of boxes with a same exponent of α
w	width of multifractal spectrum

Greek letters

δ	scale of measurement
ρ	radius of a cylindrical pore
π	constant
μ	probability for pore pixels in a grid box
α	measure of probability or singularity for a grid box
χ	partition function
τ	scaling exponent of partition function
ζ	normalized probability measure for a grid box

physical properties of porous media [16–18]. It seems that the concept of fractal allows a novel characterization of pore structure in cement paste. However, the reality is more complex. It has been revealed that the fractal dimension in cement paste does depend on the scale of measurement. For instance, Winslow et al. computed the fractal dimension to be 2–3 for a gel pore size range of 0.003–0.15 μm, which characterizes the fractal nature for internal surface of cement paste [7]; however, based on image processing technique, Lange et al. reported a constant fractal dimension of 1.25 for a size range of 0.2–2 μm, which characterizes the geometrical shape of capillary pores [8]. Such scale-dependence of fractal dimension probably implies a multifractal nature of cement paste. In essence, the concept of multifractal describes a phenomenon that the fractal dimension depends on the scale or subregion examined [19]. As a matter of fact, the multifractal property of cement paste has already been noticed, while in-depth studies were not carried out yet [8,10]. With respect to the fields of cement and concrete, Valentini et al. adopted the multifractal spectrum obtained from the digital images of cement paste as a structural probe to quantify the tendency of calcium silicate hydrate (C–S–H) gel to form clusters [20]. Carpinteri et al. confirmed a multifractal nature of concrete fracture surface, based on which an anomalous behavior of fatigue crack growth can be modeled [21,22]. In recent years, relevant studies on the characterization of porous media making use of the multifractal measure have witnessed fast developments [23–26]. It has been well documented that the multifractal analysis provides a novel characterization of the disordered porous media in terms of local singularity and scale dependence. In this regard, it shall be beneficial to apply the concept of multifractal on the characterization of pore structure in cement paste.

In this paper, we present some results about the application of fractal and multifractal analysis on simulated pore structure in cement paste. Some hydration factors are discussed, including the water to cement (w/c) ratio and the degree of hydration (DOH) of cement. It is shown that both the fractal concept and the multifractal concept are feasible in characterizing the heterogeneity of pore structure in cement paste. Moreover, it is confirmed that compared to the fractal concept, the multifractal concept allows a relatively more reasonable characterization, where the size distribution and the spatial arrangement of pore are addressed without any priori assumptions.

2. Pore structure

Various experimental techniques have been developed to detect pore structure in cement paste, such as the X-ray microtomography [3]. Besides that, as some numerical models were proposed, a virtual pore structure can be produced which simulates the realistic microscopic structural evolution during cement hydration [27–31]. Past studies have shown that these numerical models facilitate extremely to the understanding of pore structure in cement paste. Therefore, in this study, we apply one of these numerical models, i.e., HYMOSTRUC, to simulate pore structure in cement paste. With a simulated structure as input, we process the fractal and the multifractal analysis.

HYMOSTRUC is a continuum type integrated model, which constructs a three-dimensional microstructure in a way of vectors. Cement particles are simulated as spheres following a given size distribution. During hydration process, cement particles expand in a concentric way, where two types of hydration products are produced, i.e., high and low density C–S–H gels in terms of inner and outer hydration products. Specifically, the rate of hydration and the formation of inter-particle contacts are modeled as a function of particle size distribution, chemical composition, w/c ratio and reaction temperature. Two kinds of rate controlling kinetics are imposed on particles during hydration, i.e., phase boundary at early stages and diffusion controlled at later stages. In more than two decades, the HYMOSTRUC model has shown its robustness in the investigation of various properties for cement based materials. More details about the HYMOSTRUC model are available in Ref. [29]. The overall structure of hydrated cement paste consists of two parts, i.e., the solid skeleton and the pore space. In particular, the solid skeleton includes anhydrous cement grains, inner and outer C–S–H gels. With removing the solid skeleton, the left structure is the pore space.

In order to process the fractal and multifractal analysis, we discretize the original simulated continuum structure based on the following formula,

$$I(i) = \begin{cases} 0; & \text{The ith pixel belongs to the solid skeleton.} \\ 1; & \text{The ith pixel does not belong to the solid skeleton.} \end{cases} \tag{1}$$

The discretized pore space is represented by a set of discrete pixels with the value of 1 in a binary three-dimensional matrix. In this study, the spatial resolution of discretization is fixed at 1 μm, which implies that the minimum volume of pore is also 1 μm^3. As shown in Fig. 1, the numerical simulation is implemented in a cubic system with each dimension of 128 μm, i.e., $128 \times 128 \times 128$ μm^3, where the simulated DOH is 0.6 with the w/c ratio of 0.4. Some parallel simulations are also implemented to investigate some hydration factors including the w/c ratio and the DOH of cement, as shown in Figs. 2 and 3.