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Area of lineal-path function for describing the pore microstructures of cement paste and their relations to the mechanical properties simulated from μ-CT microstructures

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ABSTRACT

The pore distribution of a cement paste strongly affects its mechanical behavior such as its stiffness and strength. Porosity is an influential parameter that can be used to identify the complex pore microstructures of cement paste, but it has limitations as a scalar parameter. In this study, the lineal-path function, a low-order probability function, is investigated as a supplement or an alternative parameter for describing the microstructural characteristics of cement paste microstructures. In particular, the area of the lineal-path function is used as a measure of the pore microstructural characteristics, which can be linked with its properties.

A relatively new method for simulating crack propagation, the crack phase field model, is used to evaluate the stiffness and tensile strength of cement paste microstructures and the evaluated properties are linked to the proposed characterization parameters. The evaluation is performed on virtual specimens obtained from micro-level computerized tomography (μ-CT) images of real cement paste specimens. The validity of the microstructure-property relations obtained from the proposed characterization parameters and the crack phase field model are confirmed through the statistical analysis of dozens of specimens.

It is concluded that the correlation between the area of the lineal-path function and the mechanical properties is very strong. The parameter could potentially be used as a supplementary or an alternative parameter to describe the pore microstructures of cement paste.

1. Introduction

Concrete is one of the most widely used construction materials in general. At the same time, however, the characteristics of concrete are not fully understood, and continue to be actively investigated to either improve its behavior or to develop innovative cement-based materials. Because of the complex interactions among the constituents of composite materials, the behavior of concrete is quite complex. Furthermore, the behavior of each constituent is also complex, and it is related to the characteristics of microstructures. For example, the microstructure of hardened cement paste can be classified by multiple solid phases from hydration products and a void phase resulting from the existence of pores.

Among the microstructural features, the characteristics of pore distributions contribute significantly to the mechanical behavior of cement paste. The porosity, in the form of the pore volume fraction, was found to be strongly correlated with the stiffness and strength of cement paste [1]. The modulus of elasticity and compressive strength of cement paste is known to be related to the gel/space ratio or capillary porosity [2,3]. Although the porosity is an effective parameter for identifying the microstructural features relating to mechanical properties, additional parameters might be required to correlate the microstructures and the mechanical behavior in

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detail. For example, because the porosity is a scalar parameter, it cannot describe the characteristics of random microstructural features such as the pore distribution and clustering.

Detailed characterization of the random heterogeneous microstructures can be achieved using low-order probability functions, such as two-point correlation, lineal-path, and two-point cluster functions [4]. The probabilistic description of microstructures can be advantageous in a sense that the microstructural characteristics are stored using the probability functions that can represent key features of materials. The probabilistic description of a material not only portrays more realistic features of microstructures but can also be used to reconstruct virtual specimens for property evaluation through simulations.

The lineal-path function has been widely used to characterize random heterogeneous materials and to reconstruct virtual specimens through stochastic optimization [5,6]. The range of application of the lineal-path functions spans many engineering and natural materials with random heterogeneity. The lineal-path function has recently been applied to a lead/tin alloy [7], ductile iron [8], titanium alloy [9], the anode in a fuel cell [10], sandstone [11], and two-phase composites [12].

A probabilistic approach using the lineal-path function to characterize an entrained air void in hardened concrete was proposed [13]. More recently, the correlation between the pore system characteristics obtained from the lineal-path function and compressive strength were investigated [14]. The phases of cement paste are also characterized by the lineal-path function. Low-order probability functions, including the lineal-path function, were also found to be effective for describing the random heterogeneity in cement paste microstructures. In Ref. [15], low-order functions of capillary pores in cement paste were presented and analyzed. The dominant phases were identified using lineal-path functions while identifying the diffusivity of cement paste [16]. The thermal conductivity and air permeability in cement paste were evaluated and were related to the lineal-path function obtained from micro-level computerized tomography (μ-CT) in Refs. [17–20].

However, few in-depth analyses relating the mechanical properties of cement paste with the lineal-path function have been reported. One of the main reasons is that evaluation of the mechanical properties of cement paste at the micro-level is difficult both experimentally and by simulation. In this study, the stiffness and tensile strength of hydrated cement paste microstructures obtained from μ-CT are evaluated using simulation. The relation between the mechanical properties of the virtual cement paste specimens and a parameter from the lineal-path function is investigated. In particular, the area under the lineal-path function is selected as a random variable and is related to the stiffness and tensile strength, which are also treated as random variables.

Modeling tools to evaluate the material response of cement paste have been developed and successfully applied for property evaluation to different degrees. Recent efforts include continuum micro-mechanics-based approaches (e.g., [21–24]) and lattice modeling approaches (e.g., [25–28]). In this study, the crack phase field model [29–32], which is a relatively new approach to model crack propagation, is used as a simulation tool for evaluating the mechanical properties. In this model, a diffusive crack is represented by a model similar to the concept of gradient damage approach [33,34]. Although the crack phase field model requires highly refined mesh around the crack tip, the model is advantageous in the sense that it does not require explicit representation of crack surfaces. In addition, the model is able to effectively manage complex crack propagation including multiple crack initiation and propagation, crack coalescence, and branching through the domain of complex geometry.

The crack phase field model has been applied to a wide range of problems for the simulation of arbitrary crack propagation [33,35–41] and was also employed to simulate crack nucleation and propagation in cement paste, mortar, and concrete [42–45]. In particular, a method to determine the parameters of crack phase field modeling of concrete failure in conjunction with the digital correlation method was proposed in Ref. [44]. In this study, the crack phase field model is used as a loading tool to evaluate the mechanical behavior of cement paste under tension at the microscale. Evaluation of the compressive behavior of the cementitious materials might be more useful for practical purposes and should be more plausible to validate with experiments. However, the failure mechanisms of cementitious materials in compression are far more complex compared with those of tensile failure. Micromechanical failure modes such as shear and compression should be incorporated to evaluate the compressive behavior properly. Although some crack phase field models (e.g., [33,40]) include other failure modes in addition to tension, none of these models have been validated to identify the compressive strength of cement paste to the best of the authors' knowledge. The crack phase field model implemented and used in this study should perform the best for predicting the tensile behavior; thus, the tensile strength is investigated here.

The purpose of this study is to propose a parameter that can be additionally or alternatively used to characterize the pore distribution in cement paste. The potential of using the area of the lineal-path function in addition to porosity for the microstructural characterization of cement paste is presented by correlating the mechanical properties obtained from the crack phase field modeling.

In the next section (Section 2), the procedure for preparing the virtual specimens used in this study is shown, and the validity of the virtual specimens and characterization methods related to the lineal-path function is presented. The property evaluation using the crack phase field model, which is the virtual loading tool adopted in this study, is described next in Section 3. The relationship between the microstructure characterized by the lineal-path function and the mechanical properties from the crack phase field model is illustrated in Section 4 to show the potential of the characterization method and the loading tool adopted in this study. In Section 5, the performances of the lineal-path function and crack phase field model are discussed, and this is followed by the conclusions in Section 6.

2. Hydrated cement paste specimens

2.1. Sample preparation and μ-CT imaging

The microstructures of hardened cement paste are obtained using μ-CT as a characterization tool. One of the advantages of μ-CT is that the method can capture the microstructural characteristics relatively accurately without destroying specimens as opposed to other destructive methods such as scanning electron microscopy (SEM). The μ-CT images were obtained from a 33-keV X-ray source in a synchrotron at the Pohang Accelerator Laboratory (PAL) of South Korea. The microstructures and properties of hydrated cement paste with a water cement ratio (w/c) of 0.5 were investigated in this study. The cement paste specimens were prepared using ordinary Portland cement (Type I). After mixing the cement with water, the fresh cement paste was inserted into cone-shaped plastic tubes as shown in Fig. 1. The size of the circular cross section of the cone tubes was selected for obtaining high-quality μ-CT images, where the pixel size of a reconstructed image is 0.65 μm. The specimens were prepared and cured for 28 days until the μ-CT images were obtained.

In this study, a virtual specimen was generated from 16-bit cross-sectional images obtained from μ-CT. The value of each