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Numerical simulation of the initial particle parking structure of cement/geopolymer paste and the dissolution of amorphous silica using real-shape particles

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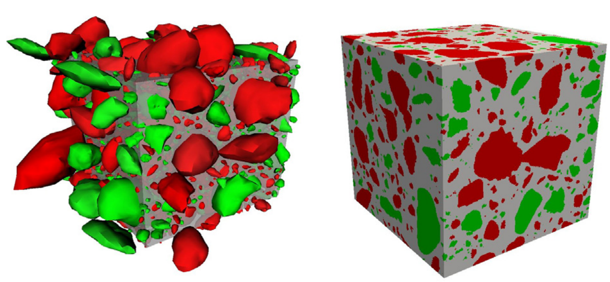
HIGHLIGHTS

- The initial particle parking structures were simulated using real-shape particles.
- The simulated initial particle parking structures were evaluated.
- The dissolution of amorphous silica was simulated by LB method and thermodynamics.

GRAPHICAL ABSTRACT



VRML image   Digital image

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ABSTRACT

Many particle-based numerical models have been used to simulate the hydration process of cementitious materials. Most of those models employ regular shape particles, like the commonly used spheres, to represent cement, slag, or fly ash, which neglects the influence of particle shape. To deal with this issue, this study extended the Anm material model and used irregular shape particles to simulate the initial particle parking structures of cement/geopolymer pastes. The irregular shapes of cement, slag and fly ash particles were characterized by spherical harmonic series. Compared to the initial particle structures simulated using spherical particles, those using irregular shape particles had total surface areas and bulk specific surface areas with up to 37.40% and 36.84% larger, respectively. However, the pore size distributions of the simulated initial particle structures did not show significant influence of particle shape. As a demonstration to illustrate the influence of particle shape on dissolution, the initial particle parking structure of amorphous silica in alkaline solution was generated using irregular shape particles, and was used as input to simulate the dissolution of silica particles. The Lattice Boltzmann method was used to simulate the transport process of aqueous ions and thermodynamics was employed to consider the rate of dissolution of silica. The dissolved fractions of silica at different temperatures in the simulations agreed well with experimental measurements. The influences of continuous stirring, concentration of alkali and particle shape on the dissolution kinetics of silica were investigated numerically.

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1. Introduction

Many particle-based numerical models have been used to simulate the hydration process of cementitious materials [1–4]. In these models, regular shape particles, usually spherical particles, are used to represent the particles of cement, slag, or fly ash. However, the real particle shapes found in cement, slag and fly ash are irregular and non-spherical due to the manufacturing processes and particle grinding methods used. Spherical shapes have the minimum specific surface area (m^2/m^3) of any closed 3D shape [5], so the greater the particle deviates from sphericity, the greater the specific surface area it has. The greater specific surface area enables the particle to hydrate faster, since hydration is a surface-controlled set of reactions [6]. It is reported that variation in particle shape influences the reaction kinetics of cement hydration [4,7].

An appropriate way to analytically characterize the shape of irregular shape particles is to make use of spherical harmonic series [8]. The spherical harmonic expansion coefficients can be obtained based on the digital images of particles from micro X-ray Computed Tomography scans [8]. Bullard and Garboczi used this technique to reconstruct real particle shapes of cement, and produced three-dimensional digitized cement paste microstructures using real-shape cement particles [7]. In their numerical model, the particles described by the spherical harmonic expansion coefficients were digitized into voxels, and then the digitized particles were parked into a predefined voxel cube. In such a way, however, the resolution of the simulated cement paste microstructure is constrained by the resolution used to digitize the particles, and the smallest particle that can be parked also depends on the digitization resolution. By implementing the spherical harmonic series, Qian et al. developed a geometrical model (denoted as the Anm material model) to park real-shape aggregates according to mortar or concrete particle size distributions [9]. The term "parking" is defined as placing a particle with random location and orientation without touching another particle [10]. After successful parking, the particle is fixed in place and the next particle is randomly parked. In the Anm model, the real-shape particles are directly parked into a predefined cube without prior digitization. Therefore, there are no limitations on the resolution of simulated initial particle structure and the smallest particle size. However, a wider particle size range implies that many more particles need to be parked to accurately represent the particle size distribution, which usually results in longer computation time. To increase the simulation efficiency, Stephen et al. improved the Anm model by integrating two new algorithms [11]. One is the extent overlap box (EOB) method that detects interparticle contact, and the other is the capability of adding a uniform-thickness shell to each particle. These two new algorithms, along with an integrated parallel processing programming interface, accelerate the particle placement/parking process.

In the original Anm material model, only one component, for example, one type of aggregates, is parked at one time [9,11]. Therefore, it cannot simultaneously park particles from binary or multiple components, for example, two types of aggregates with different particle shape databases and mechanical properties. In most cementitious/geopolymer materials, blended materials are used, such as binary-blended cement with slag, or fly ash, and binary-blended slag with fly-ash-based geopolymer paste. In this study, the original Anm material model was extended to simulate the initial particle parking structures of binary-blended systems with components chosen from cement, slag, or fly ash. In the meantime, the initial particle parking structure of cement/geopolymer paste was also simulated with HYMOSTRUC3D [4,12,13] using spherical particles for comparisons. The initial particle parking structures, simulated using real-shape particles and spherical particles, were evaluated in terms of cumulative surface area, specific surface area, and pore size distribution.

The simulated initial particle parking structure of cement/geopolymer paste can be used as input to simulate the binder reaction process. As a demonstration to illustrate the influence of particle shape on dissolution, the dissolution of amorphous silica in alkaline solution was simulated. In simulating the dissolution, this study innovatively coupled the Lattice Boltzmann (LB) method and thermodynamics to simulate the physical transport of aqueous ions and the chemical reaction between the amorphous silica and the alkaline solution. The dissolved fractions of amorphous silica at different temperatures were simulated as a function of time, and the simulated results were compared to the experimental measurements. After validation of the simulation model, the influences of continuous stirring, concentration of alkali ions, and particle shape on the dissolution kinetics of silica particles were numerically studied.

2. Materials and methods

2.1. Materials

The initial particle parking structures of six types of pastes were simulated. These six types were cement paste, slag-based geopolymer paste, fly-ash-based geopolymer paste, binary-blended cement with slag paste, binary-blended cement with fly ash paste, and binary-blended slag with fly-ash-based geopolymer paste. The particle size distributions (PSDs) of cement (type CEM I 42.5N), blast furnace slag (BFS) and fly ash (FA) are plotted in Fig. 1(a). The PSD of cement was obtained from Ref. [14], while the PSDs of slag and fly ash were similarly measured by laser diffraction in the lab. The maximum particle sizes of cement, slag, and fly ash are 104 μm, 45 μm, and 47 μm, respectively. The densities of slag and fly ash are 2.97 and 2.33 g/cm^3, respectively, measured by pycnometer in the lab. The density of cement is 3.15 g/cm^3, obtained from Ref. [14].

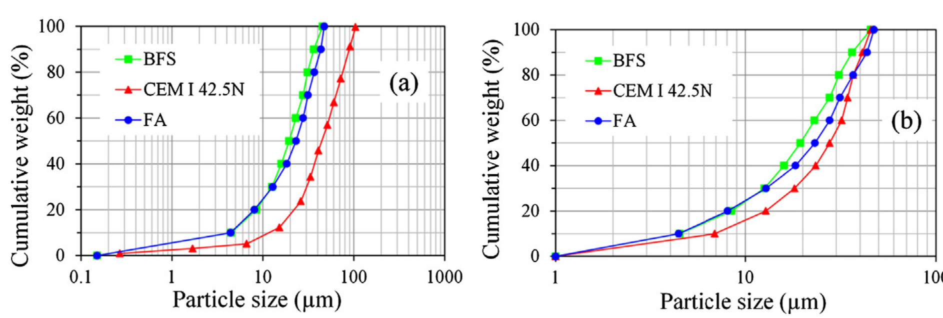

Fig. 1. (a) Experimental PSDs and (b) downscaled PSDs of cement, slag and fly ash.