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Numerical simulation of the effect of cement particle shapes on capillary pore structures in hardened cement pastes

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HIGHLIGHTS

- The evolution of capillary pore structure in cement paste is simulated with various shaped cement particles.
- Numerous algorithms are employed to determine the capillary pore structure parameters.
- Capillary pore structure parameters are influenced by geometric attribute in the early period.
- The geometric attribute of real cement particles has no significant effect on pore structure parameters in the later period.

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ABSTRACT

Cement powder shapes have a pivotal role in particle packing and microstructural development, while its effect on capillary pore structure formation in three-dimension has not been fully understood. In this study, the modified CEMHYD3D model building on previous work of irregular-shaped cement particles is firstly used to simulate the evolution of capillary pore structures in cement pastes at various water-to-cement ratios. Pore networks at different curing time and degree of hydration are extracted and visualized. Subsequently, some home-made programs for determining three-dimensional pore structure characteristics including porosity, pore size distribution, pore connectivity and pore tortuosity are carried out on these simulated pore network extractions in hardened cement pastes. The results indicate that shape-induced larger surface area in more non-equiaxed irregular-shaped cement particles can improve pore structure parameters in hardened cement pastes, but this effect will be slight in the later curing period and at a low water-to-cement ratio. In addition, the less considered geometric difference plays a role in pore structure evolution especially for extremely non-equiaxed cement particle. However, the geometric attribute has a weak effect on pore structure parameters overall. It can also be concluded that the pore-to-solid ratio is still the most pronounced influence factor for pore structure parameters in hardened cement pastes.

1. Introduction

The network of pore structure of cement paste is crucial to mass transport properties in cement-based materials, which is usually considered as indicators to assess the durability and predict the service life of reinforced concrete structures [1,2]. Different from traditional porous materials consisting of agglomerated particles, e.g., ceramics and metals, the topology of pore structure in cement-based materials is much more complicated due to the multiscale nature of microstructure and evolution of microstructure as a result of continuous hydration of cement. Pores in cement-based materials can be mainly classified into capillary pores and gel pores without a fixed critical threshold [3,4]. As cement hydration proceeds, pore space between cement particles is gradually filled by hydration products, which leads to a refinement of capillary pore structure. By contrast, the increasing C-S-H containing gel pores can result in the formation of gel pore structure with its comparatively stable intrinsic attribute of structure [5]. Compared to small and tortuous gel pores, changeable capillary pore structure plays a decisive role in transport properties in cement-based materials [6].

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Therefore, understanding the nature of capillary pore structure is of significance for investigating durability performance in cement-based materials.

It has been proved that pore structures in sintering porous materials, e.g., pore size distribution and pore tortuosity are strongly governed by performance of starting powders [7]. Particle shape, which is an important fact to be considered in starting powder, strongly influences properties of porous materials. In terms of cement-based materials, the evolution of capillary pore structure is highly dependent on cement hydration process and microstructural development. Many authors have focused on the experimental investigation of effects of raw material performance on pore structures in hardened cement pastes [8–10]. Although numerous studies concentrated on the effects of fineness (surface area) [8,9] and chemo-activity [10] of raw materials, to the authors' best knowledge, that of particle shapes on pore structures has not been yet fully explored. This is attributed to that there is no effective technique for manipulating shapes of cement particles during production process in cement industry until now. In addition, the properties of cement powder, e.g., specific surface area and particle shape, are interacted during grinding process, which is impossible to isolate the effects of specific variables in experimental investigation. Fortunately, numerical simulation may provide an alternative way to investigate the particle shaped effects on capillary pore structures in hardened cement pastes.

Before performing analysis on pore structure in hardened cement pastes using numerical simulation, the primary conundrums are to determine shaped attributes of cement particles and achieve corresponding 3D hardened cement pastes. In recent years, the sophisticated X-ray computed tomograph (X-CT) using synchrotron sources for 3D imaging with high resolution of around 1.0 μm/voxel has been employed to capture shapes of cement particles combined with spherical harmonic functions [11,12]. The reconstructed cement particles are then successfully coupled into discrete-based hydration model to simulate hydration process of this real cement [13,14]. However, the resolution of 1.0 μm/voxel is still too limited for the majority of cement particle sizes, which can well reconstruct large particles with size of over 20 μm [12]. To overcome the limitation of resolution, a locally destructive technique named focused ion beam-tomograph (FIB-t) technique with even resolution of 15 nm/voxel has been used to determine shapes of cement particles of below 10 μm [15]. The 3D cement particles are reconstructed using stacks of successive images acquired from depth profiles in FIB-t based on electron microscopy imaging and nanoscale serial sectioning provided by focused ion beam. However, as the precision of spacing between the images is difficult to control in FIB-t, it is virtually impossible to reconstruct voxel-based 3D real cement particles, which will decrease accuracy of shaped reconstruction later. Moreover, reconstructed particle library from either X-CT or FIB-t is only available for a specific reference cement due to the complex, time-consuming and prohibitive experiments.

Alternatively, modelling regular-shaped particles including spherical particles [16,17], ellipsoidal particles [18] and Platonic particles [19] are packed to represent fresh cement paste. Unfortunately, the over simplified regular-shaped particles of modelling real irregular-shaped cement unavoidably ignore the effects of shaped discrepancy on hydration in real hydrated microstructure. Furthermore, for the ellipsoidal and Platonic cement particles, the packing properties of pre-hydration microstructure can be analysed, while dynamic information in hydrated microstructure is not included. This is ascribed to that there is no approach in vector-based cement hydration model to extend spherical particles to other shaped ones for simulating microstructural evolution, e.g., HYMOSTRUC3D [16] and μic [17]. As such, it becomes more and more important to building cement hydration model based on irregular-shaped particles before investigating corresponding pore structures. Recently, our study [20] has reconstructed irregular-shaped cement particles library using central growth method on the basis of cellular automaton; these irregular-shaped particles are subsequently incorporated into discrete-based cement hydration model to investigate shaped effects on cement hydration process. The numerical simulation demonstrated that particle shapes have great influences on cement hydration: particle shaped discrepancy can not only affect cement hydration kinetics but determine setting behaviour of cement pastes. Therefore, this strong effect of cement particle shapes on hydration process leads us to consider whether cement powder shape has influence on capillary pore structure in hardened cement pastes.

This study aims at understanding the detailed relationship between cement particle shapes and pore structures in hardened cement pastes based on previously proposed cement hydration model using irregular-shaped particles. Firstly, the 3D microstructures of cement pastes are simulated using CEMHYD3D model based on different irregular-shaped cement particles generated using central growth model. The mechanism of central growth model is simply reviewed and detailed simulated cases are described in this section. Subsequently, some numerical methods for determining 3D pore structure parameters including porosity, pore size distribution, pore connectivity and pore tortuosity along with home-made programs are described in detail. Finally, the obtained pore structure parameters in cement pastes consisting of different shaped cement particles are analysed and compared to each other at water-to-cement ratios of 0.3, 0.4 and 0.5 with and without considering cement hydration kinetics.

2. Modelling of microstructural development

To directly analyse particle shaped effects on capillary pore structures, 3D microstructures of hydrating cement pastes made up of various shaped cement particles should be simulated. Our previous work has successfully proposed a 3D cement hydration model using irregular-shaped particles. This section will simply review its modelling principles and introduce some modifications in the latest version.

2.1. Irregular-shaped particle library

Different irregular-shaped cement particles can be reconstructed using a discrete-based method named central growth method. In the discrete-based method, all particles consist of a large number of fundamental voxels and their quality of reconstructed shapes is in turn controlled by the number of voxels. The core in central growth method is the growth eigenvector library which has direct relationship with particle shaped library. The relationship between one set of growth eigenvector and one certain particle shape is one-to-one correspondence. One mature particle can be obtained by voxel growth around one central voxel in a certain discrete growing space. In the growing space, the growth form is manipulated by the growth eigenvector. The value magnitude in each set of shaped eigenvector (between 0 and 100) represents growing probability around the growing point in the corresponding direction.

Fig. 1 illustrates a case of 2D evolution rules of central growth method in detail. In discrete growing space, the initial growing point is selected to be its central pixel and a certain set of growing eigenvector is also determined in advance, e.g., (9, 78, 29, 61, 14, 60, 25, 67) in this case. Subsequently, if neighbouring pixels centred on the growth point are vacant, vacant pixels around initial central pixel are activated, e.g., eight marked neighbouring pixels shown in Fig. 1a. Accordingly, the values in eigenvector belonging