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Simulating the effect of microcracks on the diffusivity and permeability of concrete using a three-dimensional model

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ABSTRACT

Concrete inevitably contains microcracks, but their significance on transport properties and long-term durability is not well established. This is because of difficulties in isolating and evaluating the effect of microcracks whether by laboratory experiments or computer simulations, owing to their complex heterogeneous nature. In this paper, a three-dimensional numerical approach to simulate mass transport properties of concrete containing microcracks is presented. The approach is based on finite-element method and adopts aligned meshing to improve computational efficiency. The mesostructure of concrete is represented by aggregate particles that are surface meshed by triangulation and porous cement paste matrix that are discretised with tetrahedral elements. Microcracks are incorporated as interface elements at the aggregate-paste interface or at the cement paste matrix spanning neighbouring aggregate particles. The main advantage of this approach is that the smallest microcracks can be simulated independent of the discretisation size. The model was first validated by comparing the simulations to available analytical solutions. Then, the diffusivity and permeability of a range of concretes containing different amounts of microcracking with increasing complexities were simulated. The results are analysed and discussed in terms of the effect of microcrack type (bond, matrix), volume fraction, width, specific surface area and degree of percolation on transport properties.

1. Introduction

The long-term durability of concrete structures is largely dependent on the resistance of the concrete to penetration of aggressive species (e.g. chloride, CO_2, sulphates, water) when exposed to its service environment. This is because most degradation mechanisms affecting concrete are rate-controlled by the transport of aggressive species through its inevitably porous microstructure. For example, the service-life of concrete structures in a marine environment is often determined by the time it takes for chloride ions to penetrate the concrete cover in sufficient quantities to induce corrosion of embedded steel reinforcement. The main transport mechanisms occurring in concrete and generally in any porous medium are diffusion, permeation and absorption. The understanding of transport processes in concrete, and how various phases in its microstructure influence transport, is absolutely critical for the development of more durable and sustainable concretes.

In practice, concrete structures are subjected to various types of actions that induce tensile stresses exceeding the tensile strength of concrete, causing cracks to form [13]. These include structural loading, thermal gradients, wet/dry cycles and freeze/thaw cycles. As such, concrete structures in service are almost always cracked. Cracks much wider than 0.1 mm cause leakage and affect the watertightness of concrete structures. Cracks also act as pathways for aggressive agents, thereby accelerating deterioration [12]. When the cracks percolate, their influence on transport far outweighs that of capillary pores because of their larger size and shorter flow lengths. Therefore, cracks not only affect watertightness, but also long-term durability of concrete structures.

Cracks larger than 0.1 mm can be controlled and eliminated by proper design and placement of embedded steel reinforcements. However, cracks smaller than 0.1 mm, i.e. "*microcracks*", are much harder to control and eliminate via structural design alone. It has long been suspected that microcracks, regardless of their origins, act as preferential paths for transport and so they may accelerate degradation processes. However, the significance of their influence on bulk transport and durability of concrete is not well understood. This is mainly because of the fact the microstructure of concrete is physically and chemically complex, multi-phase and multi-scale. The microcracks themselves are heterogeneous and spatially variable. Several phases in concrete contribute to transport and the overall property is influenced by many interacting effects, some

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of which are very difficult to isolate and quantify from laboratory experimentation. For example, one can produce and test concretes with varying amounts of microcracking by subjecting samples to controlled drying. However, this inevitably changes the concrete moisture content and degree of saturation, which also have huge influences on the measured transport properties. In this respect, numerical modelling could provide a more effective and systematic means to study these effects.

Many previous studies have examined the influence of cracks on mass transport properties of concrete such as the work of Jacobsen et al. [26], Wang et al. [37], Gérard et al. [19], Gérard and Marchand [20], Aldea et al. [6], Kamali-Bernard and Bernard [28], Picandet et al. [32], Grassl et al. [23], Jang et al. [27], Akhavan et al. [7] and Djerbi et al. [14,15]. However, the majority of the available studies relate to large (>0.1 mm) traversing cracks that go through the entire thickness of the sample. The transport properties of a medium containing such cracks can be modelled in a relatively straightforward manner because the effective property can be related to crack characteristics such as width and area using an analytical parallel model. Furthermore, most modelling work on cracks in concrete has been carried out in two-dimensions. Comparatively few studies have investigated the effect of microcracks (<0.1 mm) that are randomly dispersed in a three-dimensional microstructure. Such microcracks do not necessarily propagate through the entire thickness; in fact they are discontinuous and are more representative of those induced by shrinkage and thermal effects.

Because of the inherent limitations of analytical models, many researchers have employed numerical homogenisation schemes such as finite element, finite difference, random walk and Lattice Boltzmann for investigating transport behaviour in cement-based materials [18,28,4,2,3,41,42,16,29,17]. These methods are all very well-known approaches used in many fields to solve differential equations that govern physical behaviours, but application to study the effect of microcracks is limited. A major advantage of these techniques is that they can be explicitly coupled with digital images of the actual microstructure as input. For example, each voxel in a digital image can be considered as an element in finite element simulations. Therefore, a total and direct transference of information between the digital image and the simulation grid can be carried out [31]. However, the main disadvantage of these approaches is that the size of the numerical sample and resolution (voxel size) at which one could simulate is constrained by available computational resources. Thus, the smallest feature that can be modelled realistically is limited. This presents a major challenge for simulating the effect of microcracks in concrete because it is too computationally demanding to model a representative volume of concrete at sufficiently high resolution to capture the microcracks, in three-dimension.

An approach to overcome this obstacle is described in this study. The approach is based on aligned meshing whereby aggregate particles and porous cement paste matrix are discretised using tetrahedral elements and the surfaces of aggregate particles are triangulated, enabling these to be represented more accurately and efficiently. This has the advantage over regular meshing using cubic voxels, which inevitably represent curved surfaces as perpendicular planar surfaces. Once the three-dimensional mesostructure of concrete is established, microcracks are then incorporated as interface elements that propagate at the aggregate-paste interface (bond microcracks) and cement paste matrix spanning nearest neighbouring aggregate particles (matrix microcracks). The microcracks can be assigned with unique widths, lengths, orientation and connectivity. The advantage of this approach is that the smallest microcracks can be simulated independent of the discretisation size of the mesostructure. This approach, which was presented in a preliminary study [1], will be fully developed and tested in this paper. First, the model is validated by examining ideal cases and comparing simulations to analytical solutions. Then, the model is used to simulate the diffusivity and permeability of a range of concretes containing different amounts of microcracking with increasing complexities.

2. Methodology

2.1. Approach

An input structure of the material coupled with a transport algorithm is required in order to model mass transport phenomena. Therefore, our approach is to first generate a three-dimensional mesostructure of concrete where it is idealised as a composite of aggregate particles embedded in a porous cement paste matrix that contains microcracks. The mesostructure will explicitly account for microcracks that propagate around aggregate particles and microcracks that propagate through the cement paste matrix. Other phases such as the interfacial transition zone and air voids may also be included, but these features are not the focus of this study and so will be ignored. The mesostructure is then meshed using an aligned meshing approach and the microcracks are incorporated as either bond or matrix microcracks with different widths, lengths, orientations and degrees of connectivity. Each element within the mesostructure is assigned a transport property according to the phase that it represents. A finite element method is then applied to the entire mesostructure to simulate bulk diffusion and permeation at steady-state conditions.

2.2. Mesostructure

To generate a mesostructure of concrete, spherical aggregate particles were placed randomly in a computational cube. The aggregate particles have varying sizes ranging from 1 mm to 10 mm, and follow the Fuller-Thompson gradation. Total aggregate volume fraction ranged from 10% to 60%. An earlier study [2] showed that a computational cube that is 2.5 times the largest aggregate particle can give representative results if sufficient number of replicates is simulated and the results averaged. Aggregate particles were placed in the order of descending size with no overlaps. However, periodic boundary conditions were not applied to avoid potential meshing problems during the aligned meshing process. The non-periodic boundary conditions could produce preferential edge flow and this could distort overall results. However, our simulations (presented later) show that this effect is small and negligible for the sample size and resolution used in this study. For a 25 mm cube containing 60% vol. of aggregate particles ranging from 1 to 10 mm, around 1000 particles were required. Examples of the generated concrete mesostructure are shown in Fig. 1.

A finite element package (ABAQUS) was used to mesh the concrete mesostructure via aligned meshing. Surfaces of the aggregate particles were first triangulated, and then the aggregate particles and porous cement paste matrix were discretised using tetrahedral elements. This process is shown in Fig. 2(a) and (b). For the sake of clarity, a relatively coarse mesh of 1 mm global element size (i.e. spacing between nodes) is shown in Fig. 2. A much finer global element size of 0.25 mm was used in the actual transport simulations and each mesostructure contained $\sim 6.5 \times 10^6$ tetrahedral elements. The frequency distributions of the tetrahedral element volume and normalised shape factor for a mesostructure containing 60% vol. aggregate particles are shown in Fig. 3. The observed narrow distribution of the element volume is an important feature of the model and shows that the generated mesh is of a high quality and should lead to reliable results at a lower computational expense. The normalised shape factor is defined as the ratio of