

MODELLING THE TRANSPORT PROPERTIES OF CONCRETE FROM THREE-DIMENSIONAL MESOSTRUCTURE

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Introduction

Enhancing understanding of the link between microstructure and transport properties can facilitate the innovation of durable and sustainable concretes, and improvement in service-life modelling of concrete structures. This paper presents the development of numerical approaches to model the diffusivity, capillary absorption and permeability of concrete from its three-dimensional mesostructure. The aim is to apply these models to increase our understanding of the role of various phases, in particular microcracks, on transport properties. Concrete is a multi-phase heterogeneous material and thus, the modelling approach used must be able to capture the relevant details that influence mass transport. Analytical and empirical techniques are lacking in this aspect compared to numerical schemes such as finite element, finite difference and finite volume. In this paper, a finite difference method is used to simulate diffusion through the mesostructure of mortars and concretes. Then, a nonlinear finite element method is used to solve the set of governing differential equations for capillary absorption. Finally, a finite element approach that can potentially be used to study the influence of microcracks on diffusivity and permeability of concrete is presented.

Modelling diffusivity from three-dimensional mesostructure

In order to model transport phenomena in any material, an input structure coupled with a transport algorithm is needed. The mesostructure of concrete can be viewed as a composite of aggregate particles, bulk cement paste, ITZ, air voids and cracks. This mesostructure can either be obtained directly from appropriate 3D imaging techniques or computer simulations. Fig. 1(a) shows an example of a simulated mesostructure that is generated by considering the volume fraction, particle shape and size distribution of aggregates, thickness of ITZ and porosity of the cement paste, as a function of w/c ratio and degree of hydration [1].

A finite difference method can then be used to solve Fick's first law of diffusion coupled with mass conservation to simulate bulk diffusion. At steady state and ignoring chemical interactions:

$$\frac{\partial C}{\partial t} = \nabla \cdot (D \nabla C) = 0 \quad (1)$$

where C is the concentration of the diffusing species and t is time. The transport property of each phase is defined according to its porosity. If two particular face-sharing voxels in the mesostructure are of different phases, then the diffusivity of the connecting element is approximated as a series combination. A constant concentration boundary condition is applied to the inlet and outlet nodes. This leads to a set of algebraic simultaneous equations which can be solved iteratively. Fig. 1 (b) shows an example of the concentration distribution for a sample containing spherical aggregates at steady-state condition. Once the concentration at all nodes is obtained, the effective diffusivity D can be calculated from $D = QL/A \Delta C$, where Q is the outflow, A is the cross section area and L is the length over which the concentration gradient ΔC is imposed.

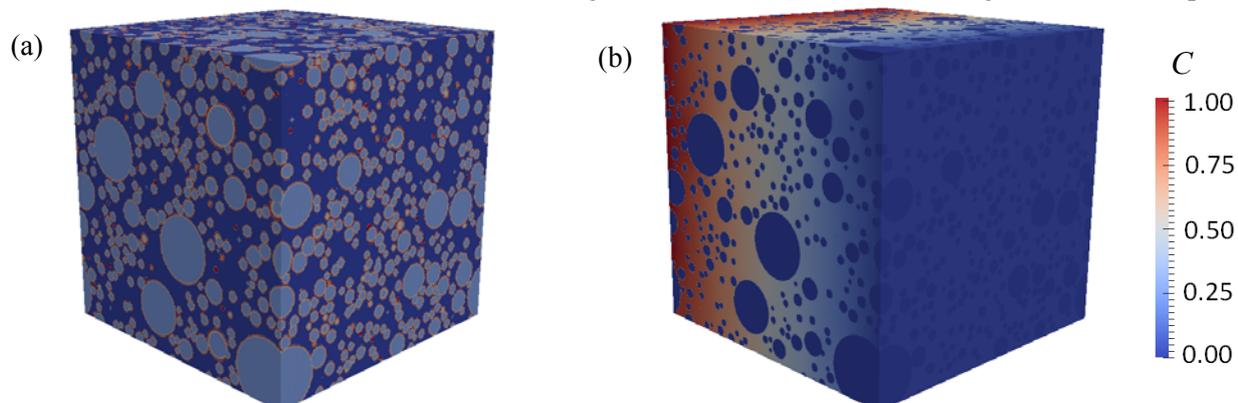


Fig. 1 (a) Randomly generated mesostructure containing 30% vol. spherical aggregates (0.15 to 2 mm, Fuller-Thompson gradation) in a 7.5^3 mm^3 computational cube (voxel size = $16.7 \mu\text{m}$). (b) Concentration profile for the same sample at 0.4 w/c ratio and 80% degree of hydration, at steady-state condition

Fig. 2 compares our simulations plotted against experimental data. The simulations were carried out at ITZ widths of 0, 25 and 50 μ m. As expected, the diffusivity ratio D/D_{cp} decreases with increase in aggregate volume fraction. D_{cp} is the diffusivity of bulk cement paste. The simulations also show that D/D_{cp} increases with increase in ITZ width. A reasonably good agreement between experimental data and simulations is found when the ITZ is between 25 and 50 μ m. The model is then applied to assess the effects of water/cement ratio, degree of hydration, aggregate size, volume fraction, shape and orientation, ITZ width and percolation on diffusivity [1].

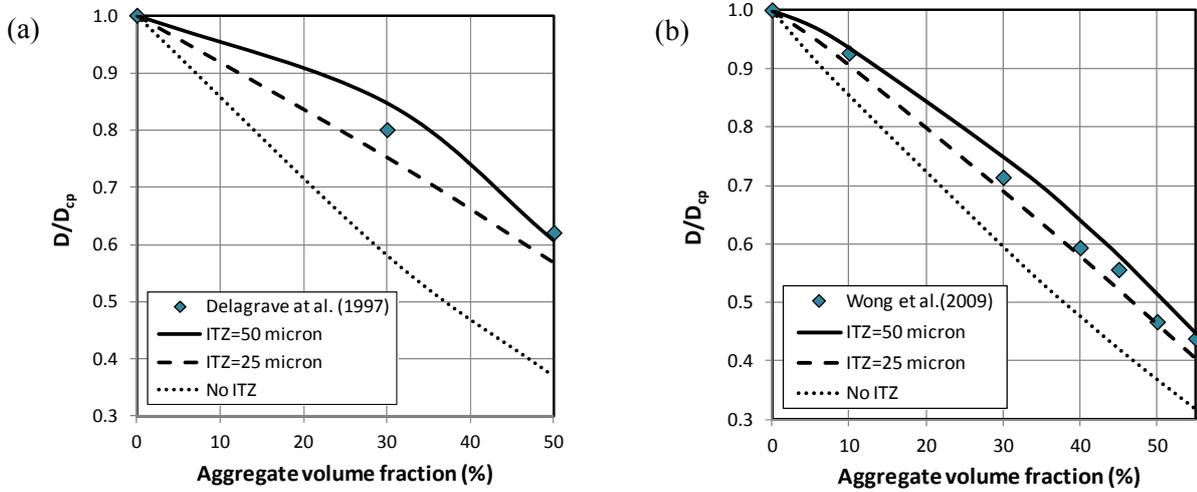


Fig. 2 Comparison of simulations and experimental data of a) Delagrave et al. [2] & b) Wong et al. [3]

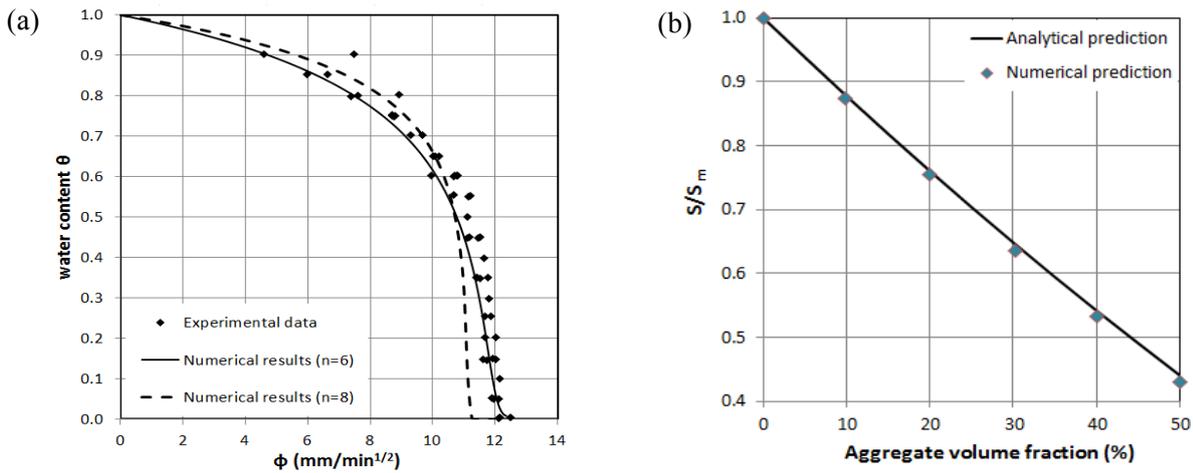


Fig. 3 Comparison of numerical results with experimental data from [4] and analytical data from [5]

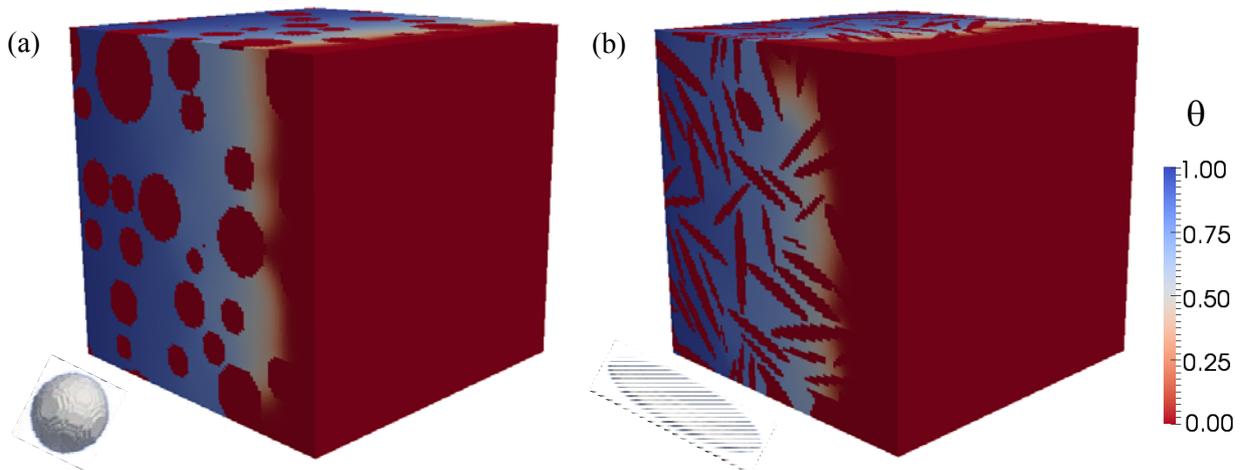


Fig. 4 Water penetration profiles at $t=16$ min for a 50^3 mm³ sample (voxel size = 0.5 mm) containing (a) spherical aggregates and (b) oblate spheroidal aggregates with aspect ratio 2:2:0.25

Modelling capillary absorption

A similar approach can be used to model capillary absorption. Here, the mesostructure is discretized as a regular cubic lattice. The lattice elements are considered as conductive "pipes" with transport properties assigned based on the phase they represent. Capillary absorption is described by a nonlinear diffusion equation, with the hydraulic diffusivity D a nonlinear function of the degree of saturation θ :

$$\frac{\partial \theta}{\partial t} = \nabla \cdot (D(\theta) \nabla \theta) \quad (2)$$

A non-linear finite element method is then used to solve the set of governing differential equations. The simulations were verified by comparing with analytical and experimental results (Fig. 3). Fig. 4 shows the mesostructure and water penetration profile for two different samples containing spherical and oblate aggregate particles.

Modelling the influence of microcracks

The main disadvantage of the regular cubic lattice models described previously is that the ratio of the computational size to the voxel size that one could simulate is constrained by computational resources. This imposes a limitation on the smallest feature that can be realistically modelled. For example, it would be too computationally demanding to have voxels small enough to represent the microcracks in a representative volume of concrete. A more efficient approach that overcomes this limitation is by aligned meshing, where discretisation is carried out using tetrahedral elements and triangulation (Fig. 5). In this way, fractures are incorporated as interface elements and explicitly considered as either bond or matrix microcracks. The smallest microcracks can be represented independent to the size of the discretisation. The microcracks can be assigned to have different widths, lengths, orientations and degree of connectivity.

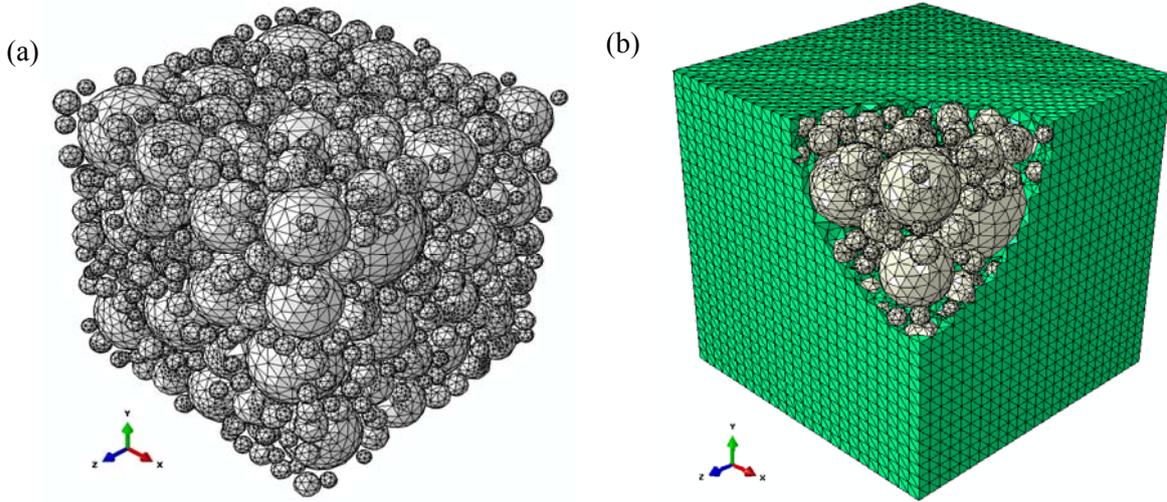


Fig. 5 Mesostructure containing 60% vol. aggregate (1-10mm) with triangulation on the surface of the aggregate particles and tetrahedral elements in the cement paste matrix

Diffusion of the cracked concrete can be modelled by considering the diffusivities of the porous cement paste matrix and cracks. Assuming that the porous matrix has a diffusivity D_m that can vary with position, the local flux \bar{J}_m in the matrix is provided by Fick's first law: $\bar{J}_m = -D_m \nabla c$, where c is concentration of the diffusing species. The conservation equation for local flux in the porous matrix at steady-state can be written as $\nabla \cdot \bar{J}_m = 0$. Assuming that the crack has a width w_{cr} and diffusivity D_{cr} (= free diffusivity D_o), the flux in the crack can be obtained by the following equation:

$$\mathbf{J}_{cr} = -w_{cr} D_{cr} \nabla_s c \quad (3)$$

The differential equations are solved using finite element, and solutions are averaged on larger scale. The total flux \bar{J} is obtained by integrating local fluxes \bar{J}_m over the porous matrix and cracks divided by the total sample volume:

$$\bar{J} = \frac{1}{\tau_0} \left(\int_{\tau_m} \bar{J}_m d\tau + \int_{s_{cr}} \mathbf{J}_{cr} ds \right) \quad (4)$$

where τ_0 , τ_m and S_{cr} are the sample volume, matrix volume and surface area of the cracks respectively. The overall flux is related to the concentration gradient: $\bar{\mathbf{j}} = -D_{eff} \bar{\nabla}c$. For an anisotropic medium, D_{eff} is a tensor. However, if the concentration gradient is imposed in one direction, the last two equations are simplified to $\bar{j}_x = -D_{eff} \bar{\partial}c/\partial x$. This approach can also be applied to model pressure-induced flow by replacing Fick's laws with Darcy's law at the mesoscale and Navier-Stokes equations at the microscale.

We have been applying this approach to study the influence of microcracks on transport properties of concrete. For example, Fig 6a shows the effect of crack volume fraction on the diffusivity of cracked concrete for the trivial case where the microcracks are arranged as two sets of orthogonal and parallel fractures. There is a good agreement between the numerical simulation and analytical solution for such a network. Fig 6b shows the influence of bond microcracks on the diffusivity of concrete. In this case, the interface between aggregate particles and cement paste are assumed to be cracked with widths ranging from 1 to 50 μm .

Other scenarios are currently being investigated to quantify the effect of microcrack parameters such as volume fraction, width, length, orientation and connectivity. To compare simulations with test data, the actual crack length and width distributions should be used as inputs to the model. The model can also be improved by coupling the transport model with a mechanical model to simulate microcrack initiation and propagation. This is an on-going task and will be reported in forthcoming publications.

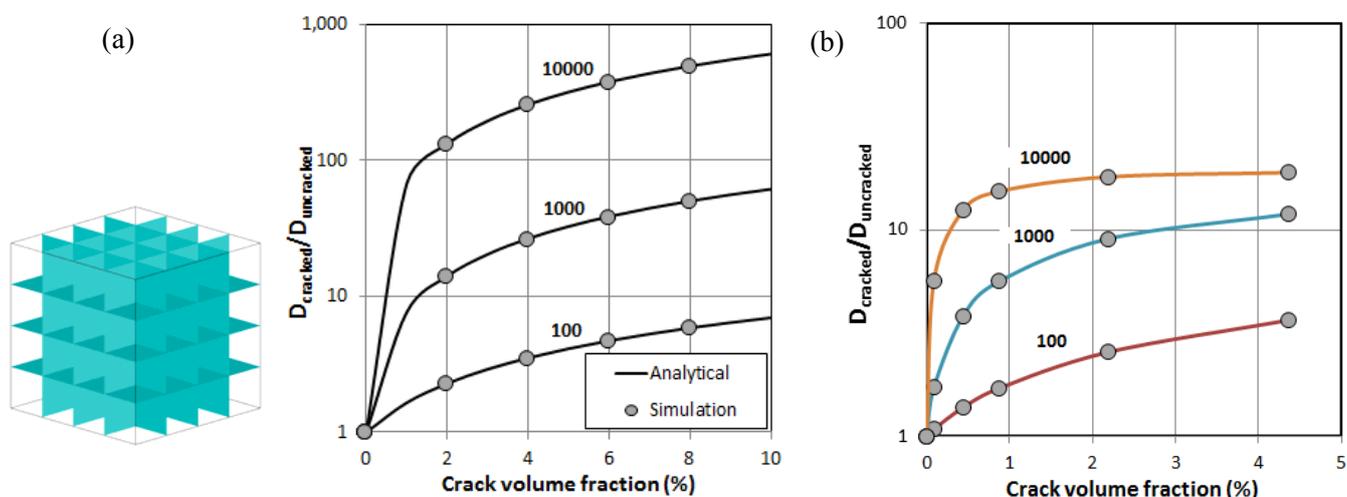


Fig. 6 Effect of a) orthogonal parallel microcracks and b) bond microcracks on the diffusivity of concrete (values on the curve are the ratio of crack diffusivity to diffusivity of uncracked concrete)

Conclusions

Three numerical schemes to model transport properties of concrete from three-dimensional mesostructure were presented. It was found that the regular cubic lattice models are appropriate for studying the effect of ITZ, aggregate volume fraction and particle shape. However, they lack efficiency for investigating the effect of smaller features such as microcracks. The aligned meshing approach where microcracks are defined as interface elements seems to be more appropriate in this case.

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