P4: The role of microcracks in concrete on water transport

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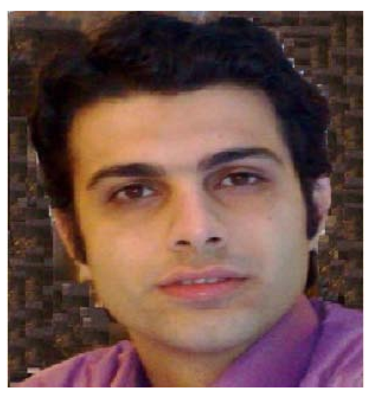


A native of Iran, Saeed Dehghanpoor obtained his MSc in Civil Engineering from École Nationale des Ponts et Chaussées, France in 2010. He started to work at Imperial College on April 11th, 2011.

Background

The microstructure of concrete and mortar is different from that of neat cement paste. The interface between aggregates and cement paste, known as the ITZ, and the presence of microcracks influence the mass transport properties of mortars and concretes. However, the role of the microstructure and in particular that of the microcracks on mass transport properties is poorly understood.

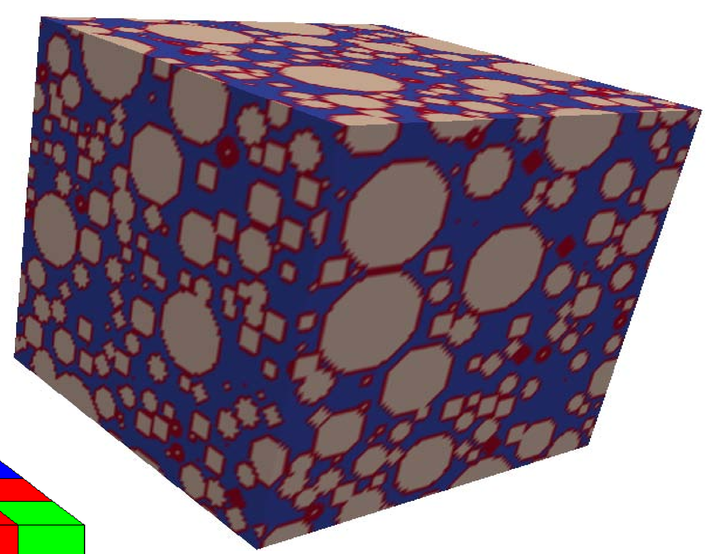
Objectives

- Develop a numerical model to predict water transport properties of concrete from measured crack network
- Apply the model to a range of samples to enhance the understanding of the role of microcracks in different transport properties
- Use the models to explore the efficiency of available methods that reduce or minimise the effect of microcracking in concrete

Approach

- Generate a mesostructure that consists of aggregate, bulk cement paste and ITZ
- Discretise the mesostructure to a three-dimensional network model
- Simulate microcracks either by applying a statistical method or by using images of real microcracks (from Project 11 & Partner Project 18) as inputs
- Model the effects of microcracks and ITZ on various transport properties
- Compare and validate results with experimental data obtained from Partner Project 18

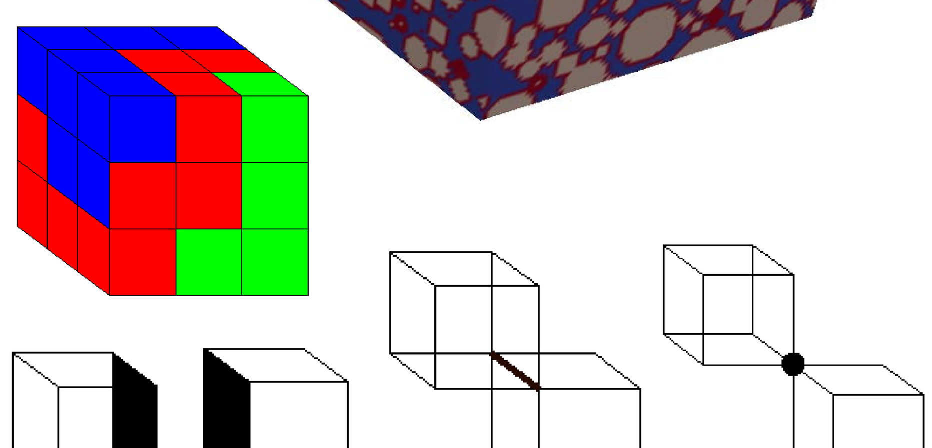
Mesostructure



To generate the mesostructure of crack-free sample:

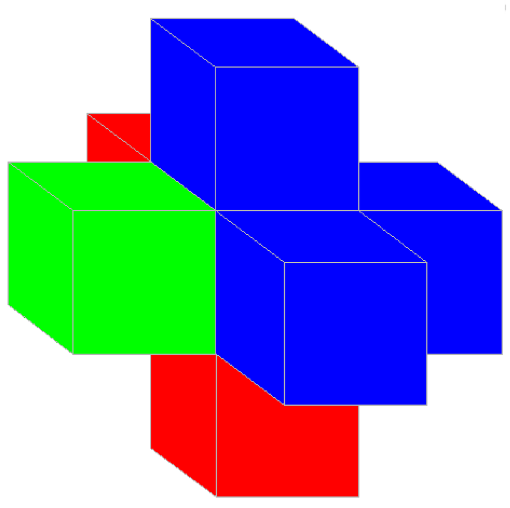
- Determine the number and size of aggregate particles from grading curve
- Place aggregates randomly
- Simulate ITZ on each aggregate
- Apply periodic boundary conditions

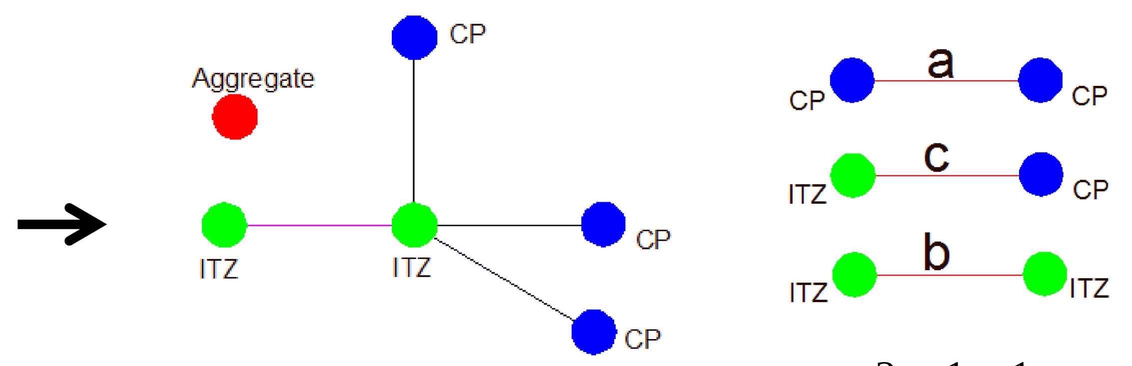
The mesostructure consists of voxels that represent aggregate, ITZ and bulk paste. Adjacent voxels are assumed connected when they share a common face and are assumed to be disconnected when they share a vertex or an edge. Transport only occurs between interconnected voxels.



(Connected) (Disconnected)

Network Model





$$\frac{2}{c}=\frac{1}{a}+\frac{1}{b}$$

The mesostructure is converted to a network model that consists of three types of elements as shown above. The transport property of these elements are represented as *a*, *b* and *c* .

Permeation and Diffusion

To simulate permeability:

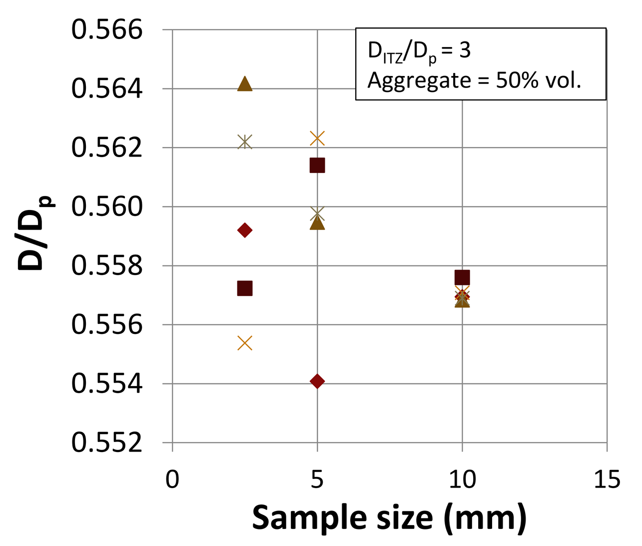
- Apply pressure gradient across the network model
- Calculate the pressure in each node by solving mass conservation equation & volumetric flow by summing the flow in the inlet elements
- Calculate permeability using Darcy's law

The process of simulating diffusivity is similar to that of permeability due to the analogy between Fick's first law of diffusion and Darcy's law. The main difference is the contrast ratio of ITZ to bulk cement paste. This has been reported to range from 10-1000 for permeation and from 2-10 for diffusion. Transport property at the scale of cement paste and ITZ can be obtained using Lattice Boltzmann (Project 3).

Results

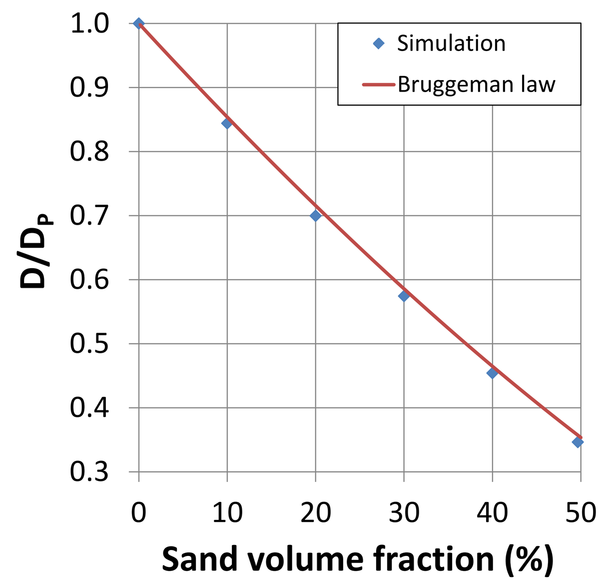
a) Representative elementary volume

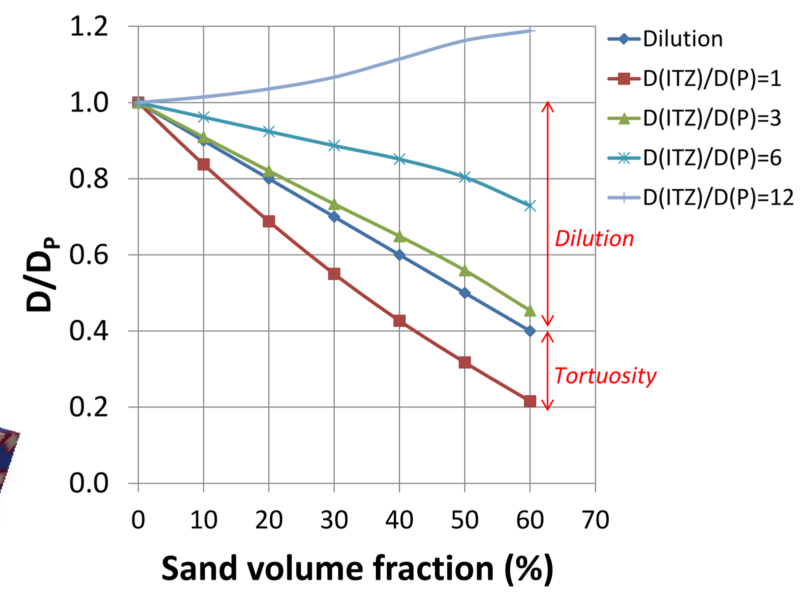
To obtain a representative estimate of the overall transport property, two options exist: simulate a large sample size at a small number of replicates, or simulate a small sample size at sufficient number of replicates. Our results suggest that a good compromise for a maximum aggregate size of 1.2 mm is to simulate a 5 mm cube at 5 replicates.



b) Comparison with analytical result

We compared the relative diffusivities for the case of $D_{ITZ}/D_p = 1$ with the well-established Bruggeman-Hanai law for the diffusivity of a composite containing spherical non-conductive particles in a conductive matrix (Bruggeman, 1935). A reasonable agreement was observed. This shows that our model can capture the effect of dilution and tortuosity.



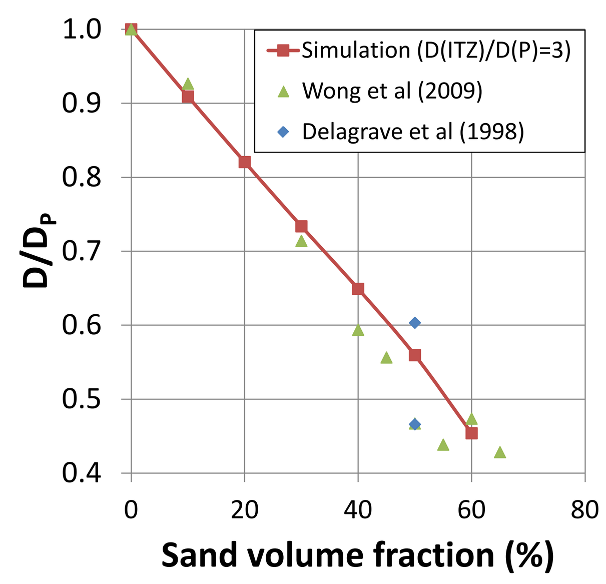


c) Effect of ITZ

The relative diffusivity (D/D_p) of mortars containing various sand volume fractions and ITZ contrast ratios (D_{ITZ}/D_p) are shown. Addition of aggregates decreases transport due to the dilution and tortuosity effect. The higher the transport property of ITZ (higher D_{ITZ}/D_p), the higher is the overall transport property.

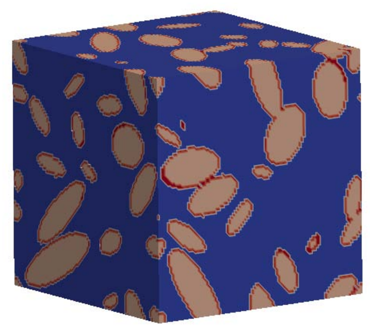
d) Comparison with experimental data

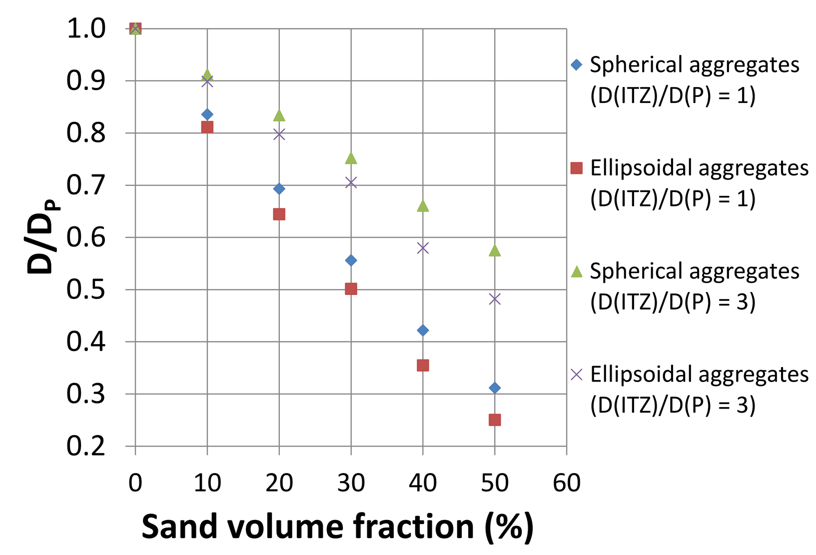
We observe that the simulated diffusivity seems to agree well with available experimental data when a 50µm ITZ width and a contrast ratio of 3 were assumed. The error in the prediction is no worse than the inherent error in the laboratory measurements. However, the influence of microcracking has yet to be accounted for.



e) Influence of aggregate shape

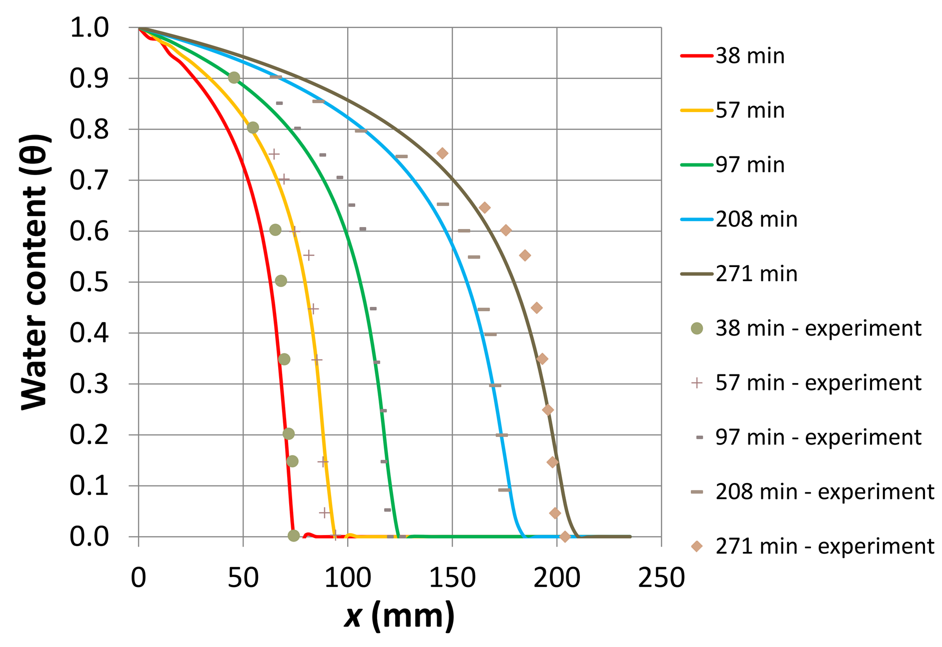
Replacing spherical aggregates with ellipsoidal aggregates increases ITZ content and the tortuosity of the cement paste. Our simulation shows that the net effect is a decrease in diffusivity. This becomes more apparent as the aggregate content is increased.





Sorption

Water transport due to capillary suction in a homogeneous mortar bar was simulated using non-saturated flow theory and the Galerkin method (Wang & Ueda, 2011). The bar was initially dry and one end was then exposed to water. The change in water content with time and depth from the exposed surface (*x*) is shown. The results suggest a general agreement with experimental data from Hall (1989).



$$\frac{AD(\theta_j)}{L}\begin{bmatrix}1 & -1\\ -1 & 1\end{bmatrix}\begin{pmatrix}\theta_j\\ \theta_k\end{pmatrix}+\frac{AL}{6\mu}\begin{bmatrix}2 & 1\\ 1 & 2\end{bmatrix}\begin{pmatrix}\frac{\partial\theta_j}{\partial t}\\ \frac{\partial\theta_k}{\partial t}\end{pmatrix}+AD(\theta_j)\begin{pmatrix}\frac{\partial\theta}{\partial x}|x=x_j\\ \frac{\partial\theta}{\partial x}|x=x_k\end{pmatrix}=\begin{pmatrix}0\\ 0\end{pmatrix}$$

Future Work

- Extend the model to the scale of concrete
- Obtain information concerning the characteristics of microcracks from Project 11 & Partner Project 18
- Incorporate microcracking into the mesostructure and network model
- Simulate the transport properties of cracked concrete
- Compare with experimental data from Partner Project 18

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