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Modeling of Concrete Microstructure for the Assessment of the Percolation Threshold of Interfacial Transition Zone

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ABSTRACT

The present contribution deals with the modeling of the concrete microstructure in order to reliably assess the percolation threshold of the interfacial transition zone. The main concept of percolation theory is the idea of connectivity. Percolation threshold denotes the volume fraction of a particular phase of a composite material at which that phase goes from being disconnected to connected (or vice versa) so that there is a change in topology of the microstructure. Percolation properties are now more or less commonly accepted as the critical geometrical and topological factors influencing the transport properties of multiphase materials [1]. Moreover, in many practical applications the structure of composite materials evolves in time so that the percolation transition occurs after an ageing time (as it is typical for cement-based materials and gels).

In the case of mortar and concrete, the transport properties are strongly dependent on the region of cement paste close to aggregate surface (typically withing 50 micrometers). This region, known as interfacial transition zone (ITZ), exhibits higher capillary porosity and larger pores than the bulk cement paste matrix [2]. These features are commonly attributed to the cement particle packing effect and the one side growth effect. However, if the ITZs do not percolate, their effect on transport will be fairly small, as any transport path through concrete would have to go through the bulk cement paste. Transport properties would then be dominated by the bulk cement paste transport properties.

The problem of the percolation of the ITZs in concrete is computationally not simple, as the geometry and topology of this phase is complex. So far, the ITZ percolation problem has been studied for spherical and ellipsoidal aggregate particles [3]. In order to get realistic results of the ITZ percolation problem, it is highly desirable to be able to perform the simulation with realistic shapes of aggregates. Note also that micrometer and millimeter length scales have to be considered simultaneously in such a study. This makes the standard models based solely on digital image processing [4] prohibitive in terms of memory requirements. Therefore the hard core – soft shell model is utilized. In this continuum

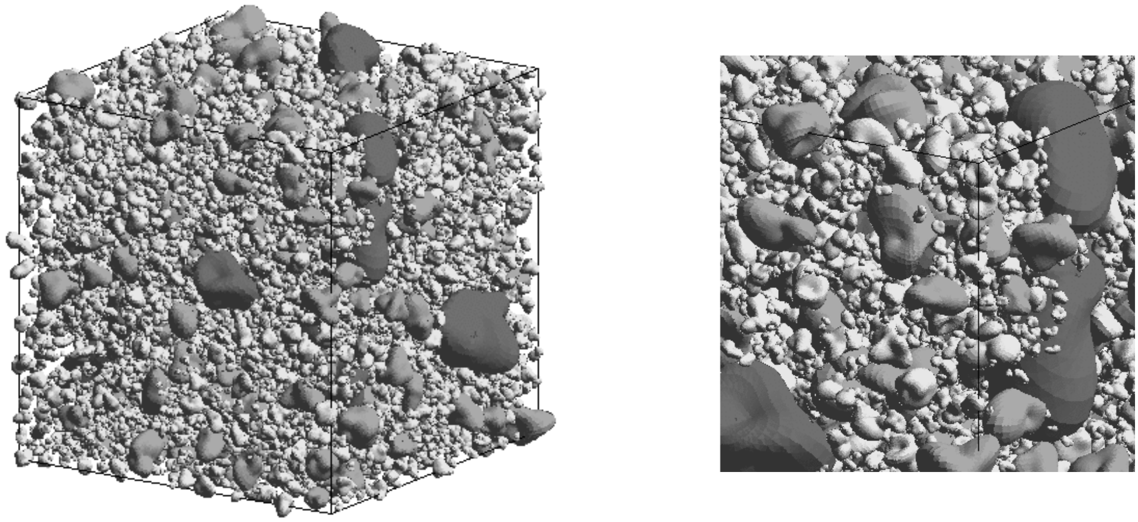

Figure 1: Aggregates packing into representative cube.

model, each aggregate particle described in terms of the spherical harmonic expansion is surrounded by a shell of constant thickness representing the ITZ. While the hard core aggregates may not overlap one another, the soft shell ITZ regions are free to overlap one another. The individual aggregate particles are randomly placed into the representative volume using a packing procedure. It starts with packing randomly generated aggregate particles, taken from a container with representative aggregate shapes, into the cubic box and then continues by expanding and shifting individual aggregate particles to make the ITZ propagate between some of the neighbouring particles. The percolation of the ITZ is verified if its propagation takes place from one side of the representative box to the opposite one at least in two directions. To obtain a reliable estimation of the ITZ percolation threshold for a particular type of aggregates and aggregates size grades, a large enough set of aggregates packs must be generated and investigated. The threshold is then calculated as the average of volume fractions from those realizations that are within the appropriately chosen tolerance from the largest volume fraction for which the percolation has not occurred and from the smallest volume fraction for which the percolation has occurred. An example of the generated concrete miscrostructure is depicted in Figure 1.

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