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Original Research Paper

DYNAMIC COMPUTER SIMULATION OF CONCRETE ON DIFFERENT LEVELS OF THE MICROSTRUCTURE – PART 2

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ABSTRACT

The establishment of an experimental basis for the dependence of a mechanical property on certain structural features (and the associated micro-mechanical properties) would require extensive, cumbersome and complicated testing: mechanical testing for defining the very property, quantitative (section) image analysis and stereological three-dimensional assessment of the relevant structural features. 'Realistic' simulation of material structure by computer would therefore offer an interesting alternative. This paper introduces the SPACE system (Software Package for the Assessment of Compositional Evolution) as the most recent development in this field. It has been developed to assess the composition as well as configuration characteristics of dense random packing situations in opaque materials. This paper presents an introduction to the system and will thereupon highlight by means of illustrative examples of typical applications on different levels of the microstructure the system's capabilities. Although only a single application can be presented in this framework, they all concern areas of major engineering interest.

Keywords: Computer simulation, concrete, material model, particle packing, stereology.

CRACKING IN CONCRETE

Recently, SPACE has been extended with the possibility to generate unstructured finite element meshes in which the material structure is explicitly modeled. Currently, only 2D meshes can be generated. Within these meshes, three components can be distinguished: aggregates, the cement matrix and the interfacial transition zone (the thin cement layer around each particle in which mechanical properties are different from that in bulk cement). In Fig. 1 part of a larger mesh is shown in which all three components can be distinguished. These meshes can be constructed because SPACE provides a full description of the material structure. Consequently, it is possible to provide the mesh generator with a function that defines the element size as a function of the distance to the nearest aggregate surfaces, for example. In this way, the interfacial transition zone (ITZ) – important for many mechanical properties in concrete – can be modeled with relative small elements while the elements within aggregates can be taken much larger.

A series of two-dimensional aggregate structures have been generated, using two different size distributions. These are denoted (A) and (B) in Fig. 3 (top). In series (A), size ranged from 1 to 4 mm, whereas in series (B), only sizes between 2 and 4 mm were considered. The particles were dispersed by the SPACE system over a square area of dimensions 14×14 mm. Thereupon, the particles were slightly eroded to create enough space between interconnected particles for the mesh generator to produce acceptable elements. The resulting areal fraction equalled 0.7 for all specimen in both series. These particle structures have subsequently been used to construct finite element meshes such as the one shown in Fig. 1 (bottom).

Static tension experiments have been simulated on these square specimens of which the boundary conditions are depicted in Fig. 2 (top). A vertical displacement was imposed on the upper side. In the present study, no periodicity of the boundary conditions is taken into account, and no periodicity of the microstructure is considered. The assumed elastic parameters and the elastic threshold of the three phases are given in table 1. In order to model microcracking, all three materials have been modeled with a nonlocal damage model, see Pijaudier-Cabot and Bažant (1987). Thus, the mathematical formulation remains well-posed in the strain-softening regime. The nonlocal damage model incorporates an additional material parameter, usually denoted as the internal length scale. This internal length scale is supposed to represent the effects of a lower scale of observation. Normally, nonlocal damage models are used at a macroscopic scale and the internal length scale is used to account for mesostructural phenomena. However, here our observations take place on the mesoscale, so that the internal length scale must be interpreted as a manifestation of a lower (say, microscopic) scale. Given the heterogeneity of, for instance, cement paste (which constitutes of hydrated grains), this seems to be a valid assumption.

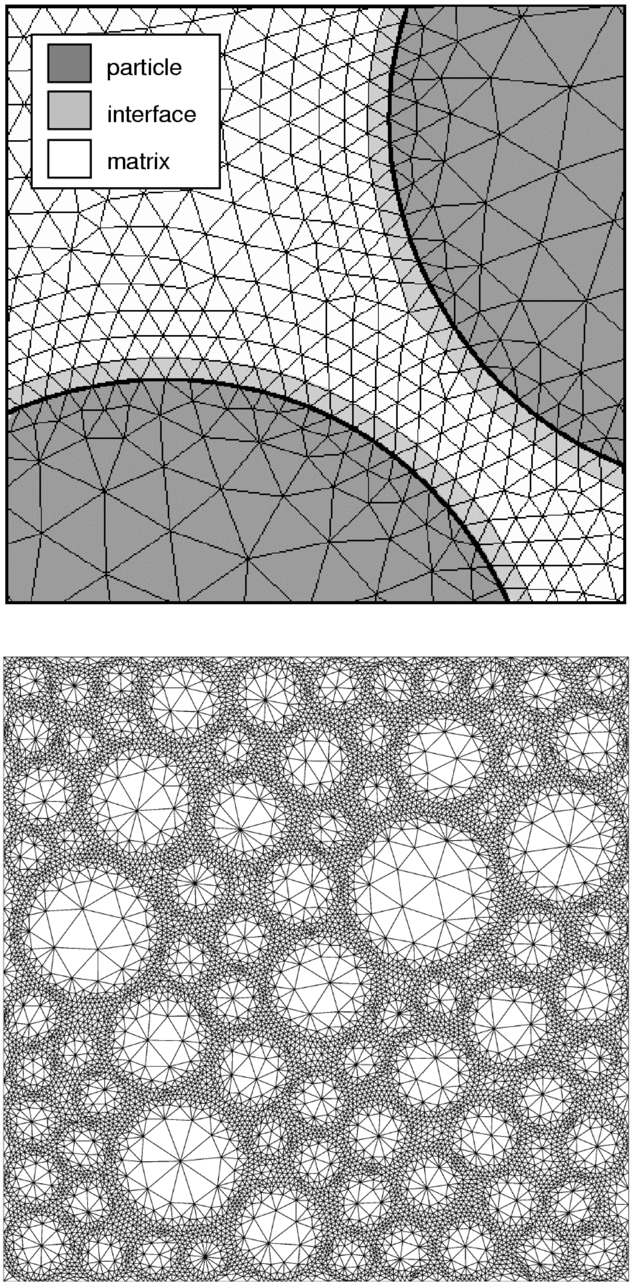

Fig. 1. *Three material components are incorporated in the unstructured finite element mesh – close-up (top) and full-size view (bottom)*

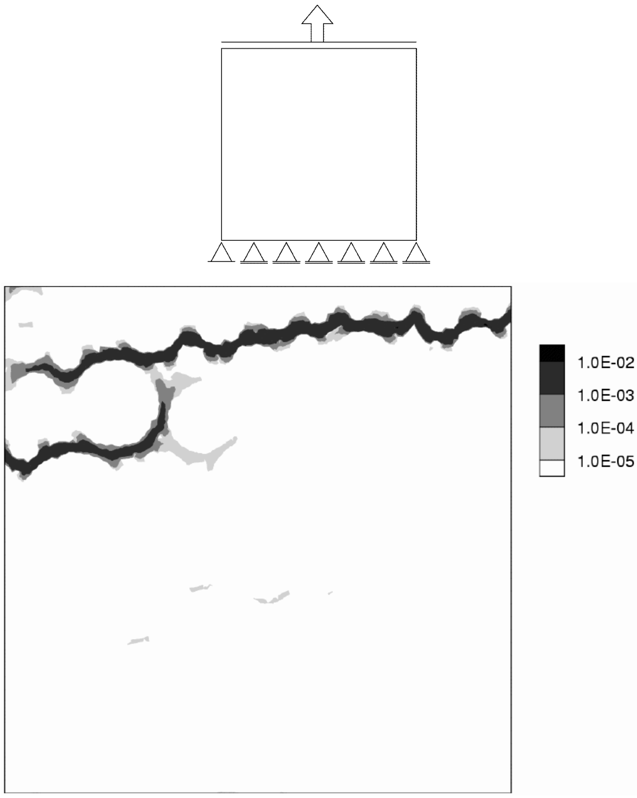

Fig. 2. *The set up of the numerical tensile test (top) and the simulated (inelastic) strain contours in one of the specimen under direct tensile stresses (bottom).*

For all three material phases, the value of the internal length scale is set equal to the average element size in the ITZ. This implies that the microcracks initiated in the ITZ will be distributed over a few elements around the ITZ. For an accurate representation of the microcrack it would have been necessary to use smaller elements, however this would have prohibited computer simulation due to storage and CPU times. For the present purpose of investigating RVEs, the relative coarseness of the finite element mesh is acceptable. In this context, it is noted that the internal length scale for the aggregates is much smaller than the applied element sizes for the aggregates, so that the regularizing effect of the nonlocal damage model would be lost in the aggregates. However, with the chosen elastic thresholds for aggregates, cracking does not occur in the aggregates. In Fig. 2 (bottom) a typical contour plot of the equivalent strain is presented.

Table 1. *The various material parameters used for the tension experiments*

component	Young's modulus [N/mm^2]	Poisson ratio [−]	crack initiation strain [−]
matrix	35.000	0.2	1×10^{-4}
ITZ	35.000	0.2	1×10^{-5}
aggregates	100.000	0.2	2×10^{-4}

As can be seen from this figure, the (inelastic) strains concentrate in the ITZ. The load-displacement curves represent global behaviour. Fig. 3 (bottom) presents the relevant curves of series (A) and (B) and the variation among the repeated simulations of series (B). Since the averages of the two series virtually coincide, the size distribution is obviously of little importance, provided total volume fraction of the mixtures is kept constant. Under the assumption that the post-peak load at complete fracture surface is primarily governed by the total surface area of the fracture plane, this finding would be in agreement with theoretical predictions, revealing indeed independence of the sieve curve (Stroeven, 2000a and 2000b). For most recent information, see Stroeven *et al*. (2002).

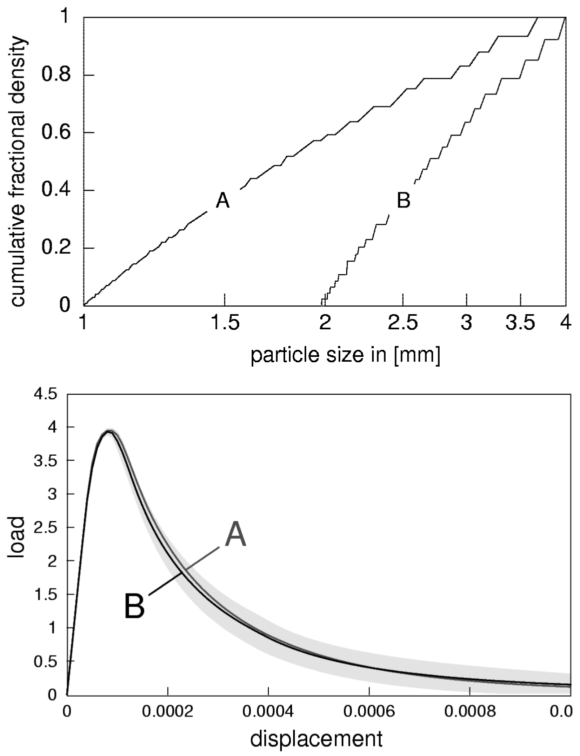

Fig. 3. *Cumulative fractional density curves of the A and B series (top) and the load-displacement curves (in relative units)of simulated response in direct tension of specimens containing aggregate with different size distribution (bottom). Scatter band of case (B) outcomes is additionally indicated.*

HYDRATION OF CEMENT

Another interesting field for application of computer-simulation systems is cement hydration. To allow for realistic explorations of the structural implications of the hardening phenomenon, 'hydration' has been implemented in SPACE. As to the validity of the approach, reference can be made to a close correspondence found between the measured strength development of hydrating cement pastes by Locher (1976) and SPACE simulations for pastes with three different water to cement ratios (*i.e.* $W/C = 0.26$, 0.388 and 0.50), assuming the strength development to be proportional to the growing contact surface area per unit of volume (Stroeven, 1999).

Preliminary results (Stroeven, 1999; Stroeven and Stroeven, 1997 and 1999b) obtained by means of SPACE simulations revealed maturity to have opposite effects on normal concretes and on HPCs; at low water to cement ratios, the ITZ thickness declined somewhat with maturity, whereas an increase was detected for normal concrete ($W/C > 0.42$, Stroeven, 1999). However, the gradient pattern of the particle packing stage is not changing *fundamentally*, as can be seen also in Fig. 4.

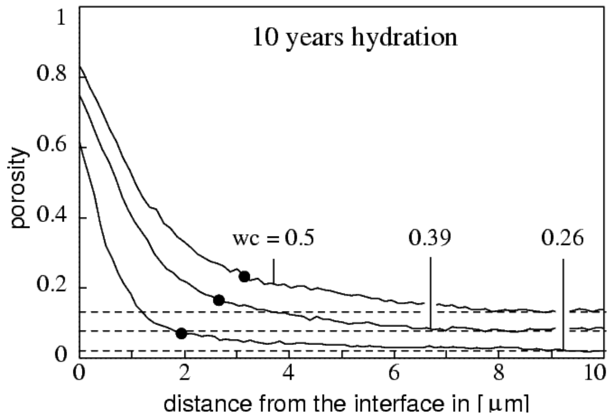

Fig. 4. *Porosity gradient in ITZ for different W/C ratios after 10 years of hydration.*

The effect of water to cement ratio on configuration is significant, as we have seen before. This leads during hardening to dramatic effects. By reducing the water to cement ratio from 0.5 to 0.4, image patterns made at 10 years hardening revealed a connected pore structure (Fig. 5 (bottom)) to transform into a disconnected network in bulk of the model material (not shown) (Stroeven, 1999; Navi and Pignat, 1996). This subject will be more elaborately discussed in a forthcoming PhD study (by Hu Jing), pursuing among other things the characterisation of pore structure by modern geometrical statistical methods of stereology and of mathematical morphology. A further reduction in the water to cement ratio from 0.4 to 0.26 yielded the number and total volume of anhydrous cement particles to increase disproportional. This phenomenon is presently subjected to a more elaborate study with the help of SPACE in the framework of a Dutch-Chinese co-operation programme on 'Modern Concrete Composites'. Distributions of pore clusters and of anhydrous cement particles showed a large degree of inhomogeneity. This conforms to experimental observations published in the literature (Scrivener, 1989; Diamond and Huang, 1998; Ollivier *et al.*, 1995). The explanation is the configuration-sensitivity of both phenomena. The higher porosity in the ITZ causes a significant reduction in the anhydrous cement content, but the gradient will still be governed by configuration. Hence, the ITZ's thickness based on the anhydrous cement content homogeneity will exceed the one for composition considerably. This is also confirmed by Diamond and Huang (1998).

CONCLUSIONS

Particle packing problems on different levels of the microstructure, ranging from maximum attainable density of gravel and sand mixtures on meso-level, to particle density distributions of cement and mineral admixtures on micro-level (as in the ITZ), can be approached effectively by the SPACE system. So far, particles are assumed spherical, so that shape effects are excluded. *Recently, the system has been developed to multi-facetted particles, allowing arbitrary shaped particles to be emphasized*. In the future, the system will be expanded to estimate mechanical or physico-chemical properties by incorporating the appropriate properties on microlevel.

The combination of a flexible software package combined with modern computer graphics techniques provides an excellent tool for simulating a variety of material systems, as shown for concrete on various levels of the microstructure. This renders possible the investigation of 'actual' structural material properties in 3-D space. The system is versatile. By changing the element properties and interactions, in principle a wide variety of engineering materials can be studied. An example in the field of cementitious materials is the effect of a superplasticizer on the distribution of cement particles in the fresh mix.

The effects of implemented mechanisms should be validated by experiments. Since this contribution aimed at illustrating the capabilities of SPACE for studying structural phenomena due to particle packing on different levels of the micro-structure, this topic was not touched upon. So far, validation has been accomplished on mono-sized particle packings compacted to maximum density, and on strength development during hydration of model cement pastes (Stroeven, 1999). For both cases, experimental data were available. The application to optimisation of gravel, or gravel and sand mixtures, presented herein, constitutes another case of validation.

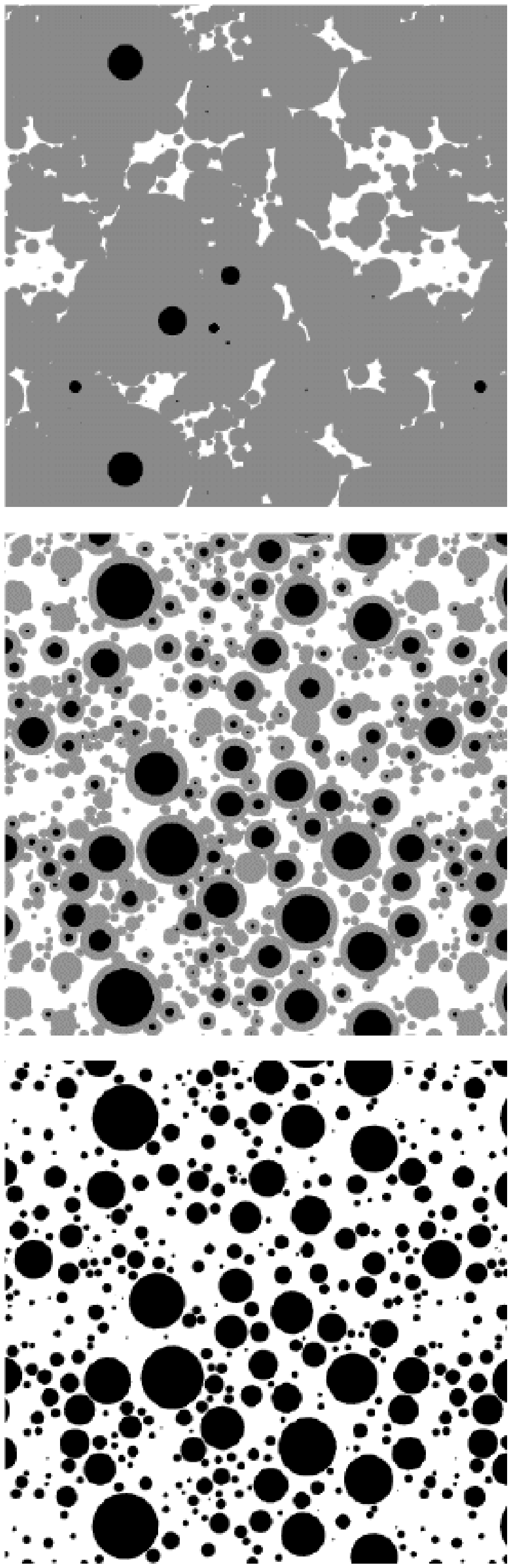

Fig. 5. *Sections of bulk cement paste with* $W/C = 0.5$ *during hydration; (top) initial stage, (middle) after 3.2 days, and (bottom) after 10 years of hydration (white areas indicate water/air, grey areas represent gel and black areas correspond to unhydrated cement.)*

SPACE simulations on model cements clearly revealed the trends due to global changes in the water to cement ratio and the cement fineness on the gradient in volume fraction of the cement particles in the ITZ. The thickness of the ITZ was in all cases only a portion of the maximum grain size of the model cement, in agreement with experimental evidences. The investigated volume fraction parameter measures *composition* of the simulated cement structure.

Contrarily, the discrimination to separate particle fractions in the SPACE approach, shows the discontinuity in particle *configuration* to extend inwards over a depth considerably exceeding the one in volume density. This phenomenon is denoted as size segregation. Since *structure-sensitive properties* depend on the details of particle packing, account should be given to a relatively wide interphase zone in assessing such material properties (like resistance to crack initiation and early crack propagation). Also on macrolevel, the discontinuity in aggregate grading (or spacing) will extend considerably more inward than estimated by volume density of the aggregate. This is in agreement with experimental evidence (Stroeven, 1973).

Simulation of configuration homogeneity for densely packed particles can not be accomplished without significant biases by conventional random generator-based systems. The paper introduces for illustrative purposes a 'global bonding capacity', as an example of a medium configuration-sensitivity property. The more dramatic effects on this bonding capacity inside the ITZ due to changes in the W/C ratio, and in the cement fineness are highlighted. Particularly under conditions relevant for HPC ($W/C = 0.2$, finest cement), the bonding capacity is *disproportional improved* due to size segregation. The associated ITZ will have a thickness of the order of maximum grain size of the cement.

The *ITZ has no distinct boundaries* due to the gradual transfer to bulk features. Deriving the thickness of the ITZ for a given composition and for the associated parameter of interest from gradient structural information would be equally difficult for experimental and simulated data. Moreover, experimental observations will suffer from a low-sensitivity (so, large scatter), and mostly be more seriously biased (Stroeven, 2000c).

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