

## Virtual Reality Studies of Concrete

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**Abstract.** The impact the computer has on materials research in the concrete technology field is discussed. The making of virtual concrete for material research purposes is relatively new. Physical simulation by discrete element methods is the most common one among the developed approaches. This paper distinguishes these approaches in two categories, the first encompassing the systems based on random sequential addition algorithms, and the second on concurrent algorithms. The latter approach provides for more realistic configuration of particles of the virtual material. This paper deals with such approaches both on meso-level, where aggregates are studied, and on micro-level, where the cement paste forms the material component of interest. Potentials are optimum mixture design and (blended) cements, which allows approaching strength as well as durability issues. This paper presents some illustrative material on these topics.

### 1. Introduction

Concrete is a particulate complex material on different levels of the material structure. The aggregate grain structure on *meso-level* is in the compacted concrete of dense random nature, at a volumetric density of about 0.70 to 0.75, depending on grain shape and on the sieve curve that crudely defines the grain size distribution function. Boundary effects due to the mould have been recognized for a long time. In or close to the jammed state, these grains form a multiple-connected network structure, providing the material in compression on engineering level with a load-bearing skeleton of mostly hard and stiff grains. The cement supposedly enrobes the aggregate grains with a thin layer, and fills the holes in the aggregate skeleton, thereby stabilizing it under loading. Crack evolution will take place in normal concrete subjected to increasing loadings, predominantly due to gradual disintegration of the bond between the aggregate grains and the cementitious matrix inside the Interfacial Transition Zones (ITZs). These ITZs, shell like zones with structure and properties deviating from those of bulk cement paste and enveloping all aggregate grains, are therefore of paramount importance in governing composite *mechanical* properties.

The fresh cement (or binder) paste has also a particulate structure on *micro-level*. Volume fraction of cement depends on the water to cement (binder) ratio, the prime design parameter in concrete technology, and varies in the practical range of concrete compositions between 0.35 and 0.55. At very low ratios, relevant for the production of (Super) High Performance Concretes (HPCs), volume percentage of binder particles can increase even to 60. Computer simulation by the concurrent algorithm-based SPACE system has revealed boundary effects in the form of structural gradients perpendicular to the aggregate grain surfaces. This holds for material density, grading (particle size distribution), internal bonding capacity, and for connected porosity, which is of crucial importance for *durability* properties of concrete. The SPACE system is able realizing this task by gradually reducing the container size in which the particulate system in a Newtonian dynamic stage is transformed from the dilute into the compacted state.

Experimental research in the two major fields of engineering interest (mechanical and durability properties) is generally time-consuming and laborious, and thus expensive. For a complete survey of the impact technological parameters exert in these two major fields on realcrete, modern virtual reality possibilities should therefore be envisaged as a highly *economic* alternative. Of course, we would like this approach also to be *reliable*. So, we require *compucrete*, produced in virtual reality, to be an adequate representation of reality (hence, of realcrete) for the *features of the material structure we are interested* in, simply because the relevant material properties under investigation rely on them. This automatically implies that this reality demand is intimately connected with the target of the research. This is a point of great concern, which is generally ignored in concrete technology.

The common virtual reality approach in concrete technology is by so-called random sequential addition-based computer simulation (RSA) systems. A range of such systems has been developed and used in concrete technology during the past 35 years, or so. It has been demonstrated convincingly by now, however, that unbiased information can be obtained by RSA systems for *composition* features only, and thus for the associated *structure-insensitive* material properties. Compucrete produced in virtual reality by such systems offers only a realistic representation of realcrete as far as information on such material characteristics is pursued. Information on *configuration-sensitive* features of material structure and on the relevant *structure-sensitive* material properties, engineers and scientists are interested in, will be biased to an unknown degree. So, this approach cannot be classified as economic either.

During the nineties of the previous century, the concurrent algorithm-based SPACE system became available for these purposes, as a preliminary terminus of earlier developments (STROEVEN, 1981, 1999; STROEVEN and GUO, 1989; STROEVEN and STROEVEN, 2001a). The only concession in the representation of reality is the use of spherical particles. The system has been extensively applied for studies on meso- as well as micro-level. Particularly, the last five years, or so, the focus was on the pore structure and on the paramount importance of the ITZ in the pore depercolation process accompanying the maturation of the material (HU, 2004; CHEN *et al.*, 2006). Gradient structures of various parameters were investigated, among which of *total porosity* and of the *fraction of connected porosity*. Even total porosity was found to be configuration-sensitive, because depending on the distance between the rigid aggregate grain surfaces. Hence, total porosity will significantly fluctuate with the size of the cement pockets inside the aggregate skeleton

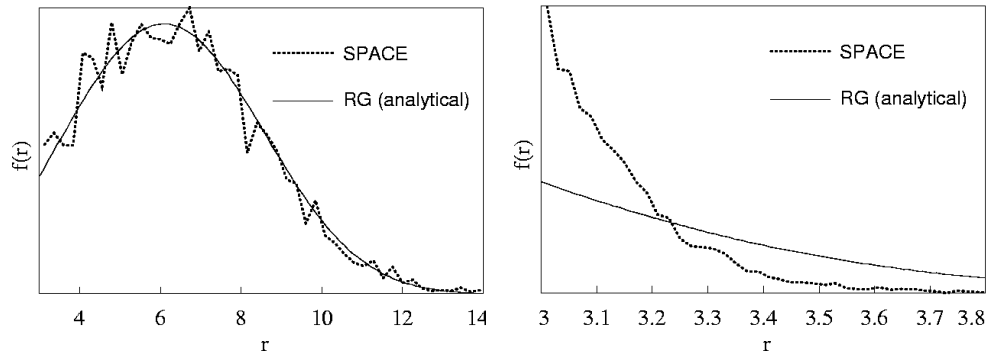


Fig. 1. Deviations between predictions on nearest neighbor density distributions,  $f(r)$ , at 1% (left) and 30% (right) by volume of aggregate obtained by a random generator (RG), respectively, and by a concurrent algorithm based (SPACE) computer simulation system (STROEVEN and STROEVEN, 1996).

structure. The connected fraction of porosity was at the ultimate degree of hydration limited to the immediate neighborhood of the rigid grain surfaces, forming a spatial interconnected network structure providing for concrete's hydraulic features.

At the moment, an even more advanced system is in development, the HADES toolbox. It is based on artificial grain shape. In a running study, optimization of aggregates of various origins will be assessed with this system. Additionally, undesirable compaction-induced grain interferences evoked by the compaction process (e.g., Brazilian nut mechanisms) can be investigated. This paper will go into relevant details of the abovementioned virtual reality studies of concrete at different levels of the microstructure. Further, it will start by discussing first the relevant methodological and scientific principles that would guarantee such approaches sharing economy and reliability. Description of our research work in this paper aims at a multi-disciplinary audience interested in computer simulation in engineering.

## 2. Virtual Concrete

How do we do that, making concrete in virtual "reality"? What characteristics of the complex, particulate material should be incorporated in this so-called *compucrete*? Such questions must have been at the minds of those coming up with the first systems in the 70s of the previous century, such as that of ROELFSTRA (1989), which formed the starting point of the numerical concrete concept of ZAITSEV and WITTMANN (1977). Basically, these and later developed systems in concrete technology rely on random sequential (particle) addition (RSA) algorithms (DIEKÄMPER, 1984; BREUGEL, 1991; BENTZ *et al.*, 1993; MEAKAWA *et al.*, 1999). In RSA systems, particles are placed proceeding from large to small on preconceived Poisson field positions, generated by a random generator algorithm (RG). Violation of physical conditions by overlap leads to *rejection and re-generation*. So, part of the Poisson field positions cannot be exploited, since spacing with other points is insufficient. The consequences are that, firstly, new positions should be randomly assigned

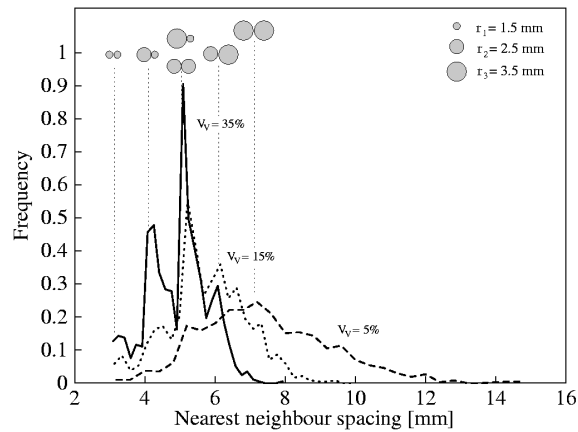


Fig. 2. Nearest neighbor distributions in aggregate mixtures composed of three particle sizes (3, 5 and 7 mm) at total volume contents of 5, 15 and 35%. At increasing volume density, particle clustering becomes an apparent phenomenon (STROEVEN and STROEVEN, 2000).

to remaining particles until overlap is avoided. This is a time-consuming process, whereby the number of re-generations dramatically increases when the volume fraction is approaching a level of only 35%. In WILLIAMS and PHILIPSE (2003) an upper limit of 38.5% for spherical particles is mentioned, which is in qualitative agreement with BALLANI (2005) where in most cases the production of computer concrete with 40% spherical aggregate failed. So, *practical* arguments plea for application to low density grain mixtures only. Secondly, instead of having series of particles close together in compcrete, in conformity with Poisson point processes, on average a more uniform dispersion is obtained (Fig. 1).

Clustering, a *natural phenomenon in particulate matter* (STROEVEN, 1973), is therefore very poorly represented by RSA systems. On the contrary, the concurrent algorithm-based computer simulation system that will be introduced later imitates the production conditions of concretes and has been demonstrated realistically incorporating the clustering phenomenon in compcrete (Fig. 2). More generally speaking, particle dispersion in SRA-based virtual concrete is seriously biased, because it does not constitute a realistic representation of the realcrete.

For a long period of time, concrete was considered a relatively simple material, although “concrete was never simple, we were” (GILKEY, 1950; STROEVEN, 1973). Neither did the relatively low price of the material form a strong impetus for material optimization studies, because research on macroscopically heterogeneous opaque materials like concrete requires large samples, is inevitably laborious and time-consuming, which makes it extremely expensive.

Instead, it was cheaper to systematically over-design concrete structures. This economy requirement also demands attuning the virtual reality of compcrete to the research purposes. Modeling pursues a schematization of reality with operational potentials. This points to the *intimate relationship between the type and degree of schematization and the*

*objectives for the appeal on the operational potentials.* We do not have to schematize all aspects of the inherently complex system that concrete definitely is, but only those relevant for obtaining this unbiased 3D structure information on which the aspect of material performance relies. A complicated task, anyhow. However, we might discover that at least some of our questions deal with aspects of material performance that have a low structure-sensitive nature. Hence, the *schematization of reality* is **not very demanding** for the simulation system when the researcher is targeting material density, or volume fractions of composing compounds of the material. These are *composition* characteristics of material. The associated material properties completely depending on composition are denoted as *structure-insensitive* properties (like mass, or approximately, Young's modulus). When investigating particle spacing, or local grading characteristics, one is dealing with *configuration* characteristics of the material. The associated material properties are referred to as *structure-sensitive*. So, the *schematization of reality* is **quite demanding** for the simulation system when the researcher's focus is on structure-sensitive properties. Compucrete should be more sophisticated in such cases, because configuration of grains, the so-called group effect, will influence these properties.

Available physical computer simulation methods for forming granular packing of hard particles can be classified, therefore, in two distinctive groups. Most computer simulation systems in concrete technology fall in the first category. They generate granular packing of spheres or particles with other idealized shapes by *random sequential addition*, RSA. The second group, based on so-called *concurrent algorithms* (CA), involves the densification of a fixed number of particles. The strategy to solve the overlap problem is either of static or of dynamic nature. In both cases, the container size is initially enlarged so that all particles can be positioned at the Poisson points. Thereupon, the container size is gradually reduced and the particulate system squashed. The mechanical contraction in WILLIAMS and PHILIPSE (2003) is a *static solution*, which involves local shifting of particle positions to eliminate overlap. The system is also developed for spherocylinders up to an aspect ratio of 160 (simulating fibre reinforcement). Jammed states were found for spheres at 63.1% and for spherocylinders with an aspect ratio of 0.4 at 69.5%. The SPACE system that has been developed at Delft University of Technology realizes the compaction by a dynamic algorithm. The dynamic stage is supposed to imitate, moreover, the production stage of the material. The forces added to the particles can be manipulated, so that "sticky" particle contacts (or particle repulsion) during the production of the model material can be simulated. Also gravity effects can simply be included. This dynamic (Newtonian) simulation mechanism has no significance after completion of the simulation, hence, is not connected with the rheological properties of the cementitious model material (STROEVEN and STROEVEN, 2001a). SPACE is based on spherical particles only. However, at present a new system is in development allowing the use of arbitrarily shaped particles (the so-called HADES toolbox, introduced later). This is to account for particle shape effects that seem to have more serious impact on packing than so far assumed in concrete technology. An earlier system with a dynamic solution in molecular dynamics is referred to in WILLIAMS and PHILIPSE (2003).

The compucrete is produced in limited quantities in cubic moulds. Basically, containers with *rigid* walls are used, or with so-called *periodic* boundaries. The first situation conforms to a molded aggregate, or to cement pocketed between surfaces of aggregate

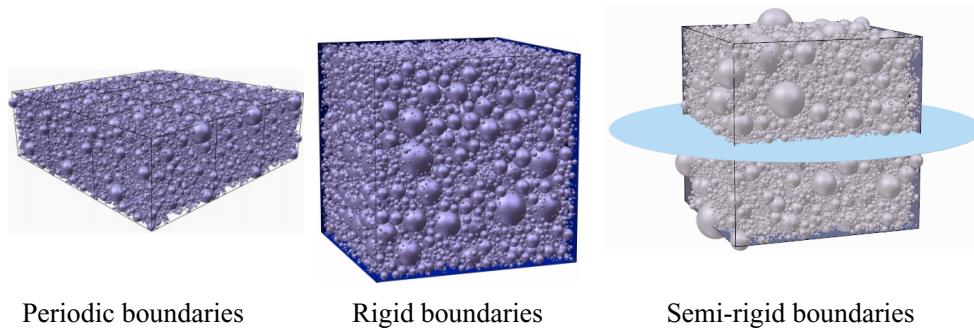


Fig. 3. Fresh model cement paste structures produced with different boundary conditions.

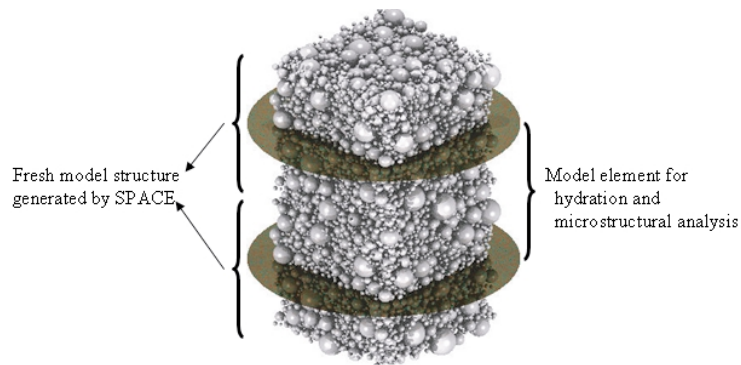


Fig. 4. Fresh model cement paste structure with semi-rigid boundary conditions.

grains. The second type of boundary conditions is used to simulate bulk material. Recently, we have used a mixed situation, whereby two rigid surfaces were combined with four periodic ones. This is constructed from a cube with periodic boundaries in which halfway a rigid surface is embedded (Figs. 3 and 4).

How to design the size of such elements in order to obtain representative information? Here we touch the materials science concept of stochastic heterogeneity. Stochastic heterogeneity declines differently for different independent descriptors of material structure. At an acceptable lower limit of scatter, the relevant parameter is defined as homogeneous. This is achieved for a particular size of the material volume, the so-called *Representative Volume Element* (RVE). Alternatively, when parameters are studied by way of quantitative image analysis, the *Representative Area Element* (RAE) can be defined similarly. The linear dimensions of the *representative* volumes or areal elements of virtual concrete, on which studies should be based, increase with rising degree of configuration-sensitivity. Nevertheless, sub-representative sample designs can still be employed in composition cases, since the probability density function of the composition parameter obtained on

Table 1. Particle spacing parameters on different sampling levels (all dimensions in mm).

Container size	Mean spacing	Mode spacing
253	0.1083	0.0751
92.6	0.1062	0.0993
46.3	0.0989	0.1640

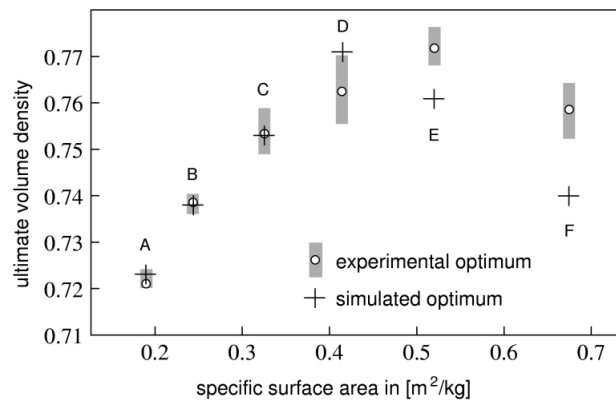


Fig. 5. Comparison of the density at the jammed states of different mixtures of river gravel aggregate compacted in standard cylinders, and of SPACE-generated spherical aggregates with similar grading characteristics. Correspondence is satisfactorily.

series of “similar” virtual concrete samples will be of Gaussian type. So, the average value is an unbiased estimate of the population mean. This is fundamentally different for configuration-sensitive parameters for which the probability density function will be skewed to the left. The curve’s mean or mode (=top of curve) parameters will undergo shifts when the sample size is changed (Table 1). So, they are *biased estimates* of population values, i.e., of virtual samples with representative linear dimensions. These materials science principles therefore govern economy and reliability of the virtual concrete for the pursued goals.

### 3. Virtual Reality Studies by SPACE on Mesolevel

SPACE-generated virtual compounds of spherically shaped aggregates packed into the jammed state were compared with experimental results. Densities varied between 72% and 75%, depending on the respective sieve curves. Results were found in very good agreement with experimental observations on aggregates of fluvial origin with similar sieve curves and compacted in standardized way in cylindrical moulds (STROEVEN and STROEVEN, 1999, 2001b), as shown in Fig. 5.

In another study (STROEVEN, 1973), concrete mixtures were composed of a fine

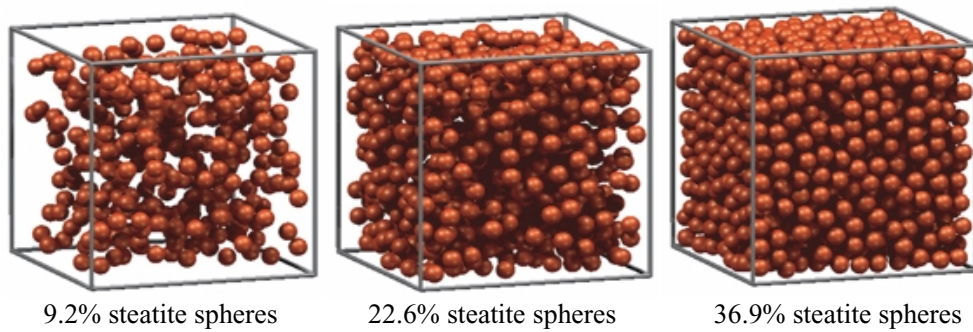


Fig. 6. Three compcrete specimens with indicated compositions as produced by SPACE.

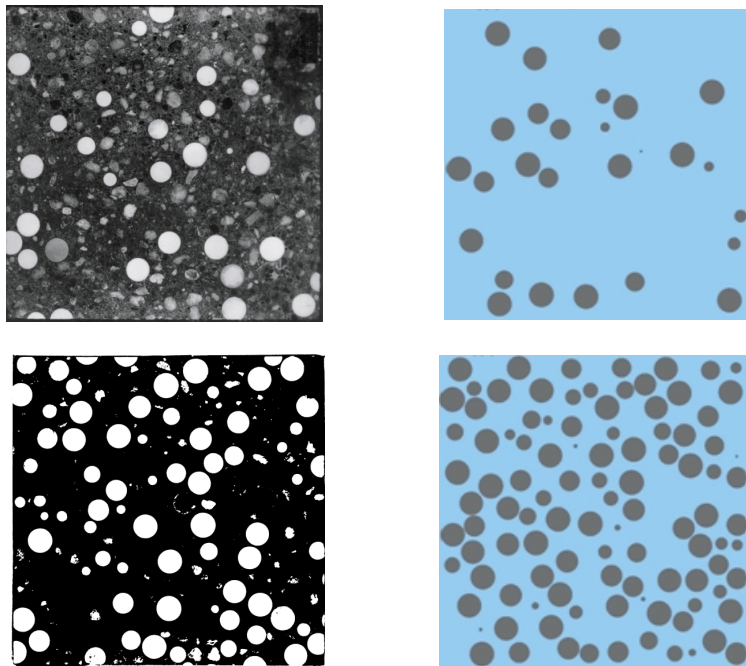


Fig. 7. Section images of realcrete (left) and compcrete (right), showing clustering tendency at increasing volume fraction of coarse aggregate (top: 9.2%; bottom: 36.9%).

aggregate (called sand in what follows) of which all grains passed through the 11.2 mm sieve and different amounts of 16 mm mono-size spherical ceramic (steatite) aggregate. The resulting sieve curves fall roughly inside the area indicated in the German building code of those days for proper mixtures (ROTHFUCHS, 1962). The three mixtures are based



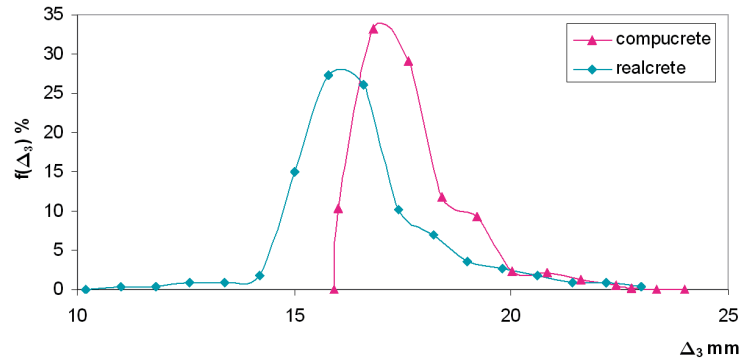


Fig. 8. Spatial distribution in realcrete and compucrete of the nearest neighbor distance,  $\Delta_3$ , for the intermediate mixture with 16 mm mono size spherical aggregate.

on 10%, 30% and 50% by weight of steatite in the total aggregate, respectively. Ratios of sand to cement (4.4) and water to cement (0.5) were similar for all mixtures. Three 250 mm concrete cubes were prepared per mixture, in addition to series of other specimens for a variety of different tests. Boundary layers with a thickness of about 1.5 times the maximum grain size were removed from all sides to yield 200 mm cubes for the investigations. One of the 200 mm cubes per mixture was serially sectioned into tiles with a thickness of about 11 mm, so that 34–38 images were obtained per cube. Firstly, all section images were subjected to stereological approaches for quantitative image analysis, exclusively focusing on the amount and the distribution of the steatite grains. This provided information on composition as well as on configuration of the particle sections. Secondly, the spatial position of all steatite spheres was reconstructed from perimeter measurements per grain section and information on the respective positions of the section images in the cube. This allowed for a 3D assessment of the nearest neighbor distribution in the cube.

Two-phase systems were generated by SPACE, consisting of mono-size 16 mm spheres and a uniform matrix. For that purpose, the appropriate volume fractions of aggregate were calculated from the weight proportions mentioned. This resulted in 9.2%, 22.6% and 36.9% by volume of aggregate per mixture. Next, the particle numbers per cube were calculated and subsequently dispersed in the dilute state in containers significantly exceeding the size of the cube used in the experiments. Thereupon, they were slowly compacted with the dynamic concurrent algorithm in SPACE to the 200 mm cube size and the proper compositions, shown in Fig. 6. It should be reminded that the major difference with the experiments was that a uniform matrix replaced the sandy mortar.

The most obvious way of comparing *realcrete* (experimental mixtures) and *compucrete* is by way of the visual impression section images, experimentally obtained by sawing the specimens into slices. The successive section patterns fluctuate of course in the experimental as well as in the simulation setting. Nevertheless, in both cases we see *particle clustering* reflected in the 2D section images (Fig. 7).

The toughest test on reliability of the virtual reality is by comparing the nearest

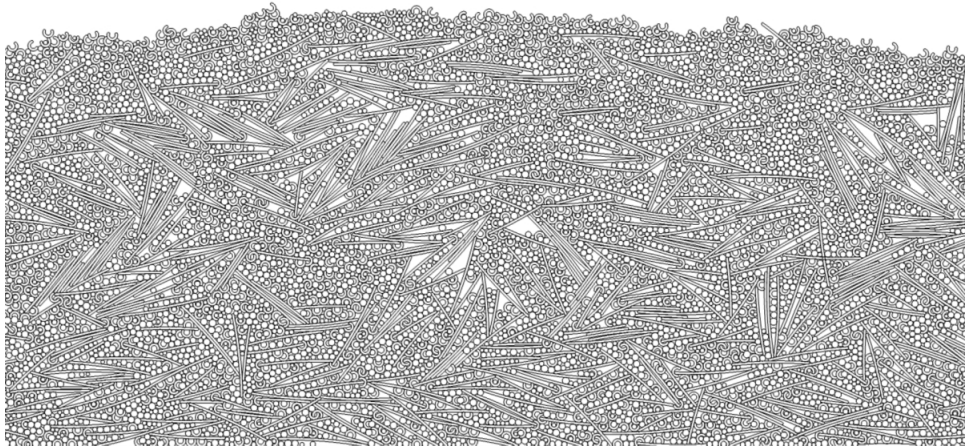


Fig. 9. A two-dimensional dense packing of a variety of objects.

neighbor distribution of particles in cubes,  $f(\Delta_3)$ , since this is a structure parameter of high configuration-sensitivity. In the experimental approach, the thickness of the serial slices obtained by sawing was measured and the average thickness of the saw cut calculated. Next, three widely spaced points on each perimeter of all particle sections were manually recorded on real size images (i.e., coordinates were recorded on an underlying measuring tablet upon making a slight manual imprint). A reconstruction algorithm based on Pythagoras' rule, the measured slice thickness, and the estimated average saw cut thickness, was employed for the derivation of sphere center positions and radii. The differences in Fig. 8 between information derived from *realcrete* and *compucrete* is primarily due to the relatively low sensitivity of the *realcrete* approach, yielding the small tail at the left, and the significant portion of spheres with a radius slightly less than the actual one of 8 mm in the experimental approach. Hence, the *compucrete* information is more realistic than that of the *realcrete*! However, similarity is quite convincing (STROEVEN *et al.*, 2007).

#### 4. Recent Methodological Developments

Because inter-particle contacts in SPACE were impulse-based, they occurred in an infinitesimal small timeframe. Hence, forces between particles could not exist. As a consequence, force-based experiments, such as densification under pressure, could not be performed. Moreover, SPACE limited the particle shape to spheres only. For that reason a new discrete element package, called HADES, has been developed. With this package, particles can be of any shape and contacts are force-based rather than impulse-based. The surface of objects is no longer described by a mathematical function (such as in case of a sphere), but by a set of interconnected surface elements. In this way any shape can be described. Figure 9, showing a two-dimensional dense packing of a variety of objects, illustrates the versatility of this approach.

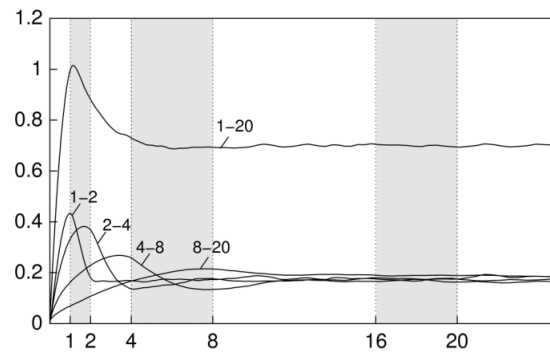


Fig. 10. Size segregation in the fresh state in model Portland cement with grain sizes between 1 and 20  $\mu\text{m}$  (so, e.g., 1–2 means all particles in the 1 to 2  $\mu\text{m}$  range). The aggregate grain's specific surface area is plotted in relative terms along the vertical axis. Distances to the interface surface are indicated on the horizontal axis in  $\mu\text{m}$ .

Particle densification by shaking, flow, or impact constitute but a few examples of the simulation possibilities. Three-dimensional simulations are possible as well. The MPG movie *BrazilianNut.mpg* demonstrates that it is possible to simulate typical dynamic granular effects such as size segregation by vibration (the so called Brazil nut effect). The second movie *Impact.mpg* illustrates that it is possible to simulate particles packing subjected to high stresses, something that was not possible with SPACE.

##### 5. Virtual Reality Studies by SPACE on Microlevel

Simulations can be realized in containers with periodic, rigid and mixed boundary conditions. Rigid surfaces allow the study of gradient structures in cement particle packing in the fresh state, so-called *size segregation*, as shown in Fig. 10. Size segregation can also be expressed in other geometric terms, like volume fraction or spacing of grains. The general pattern is that of the smallest particles migrating closest to the interface surface. The next largest fraction has its highest volume density a bit further away, and so on. The mould disturbs the aggregate composition equally on mesolevel, of course (STROEVEN, 1973). The size segregation phenomenon is at the basis of the formation around the aggregate grains of ITZs, which have paramount impact on mechanical and durability performance of the material. The size segregation mechanism has been successfully exploited to explain the importance of the gap in particle size ranges of Portland cement and mineral admixture on the strength efficiency due to cement blending (DAI *et al.*, 2005). Of course, this gap-grading phenomenon can only fully manifest itself when proper production conditions (workability and compaction energy) are provided, as revealed by Fig. 11. The size segregation phenomenon, which is only partially reflected by Fig. 10, yields gradient structures in the fresh state (such as displayed in Fig. 11) that are at least qualitatively pertaining into the hardened state. This is illustrated in Fig. 12 for the mean free spacing.

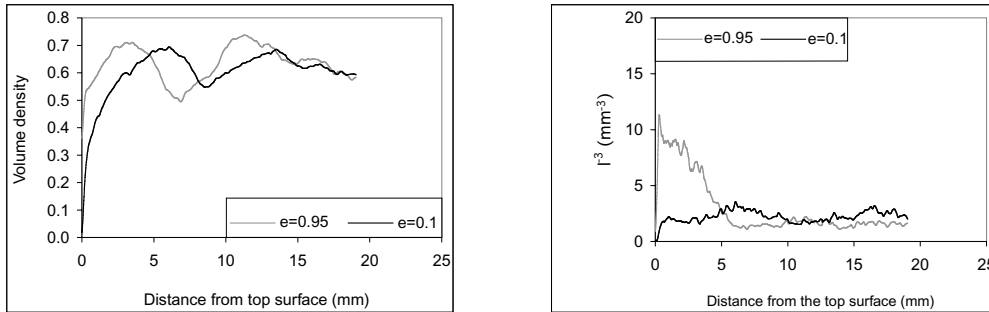


Fig. 11. Effect of workability conditions on density (a) and internal bonding capacity (b) of fresh binder with discontinuous grading. The parameter  $e$  represents in SPACE the energy dissipation during compaction. High value of  $e$  corresponds with better workability. Internal (van der Waals) physical bonding is supposedly proportional to  $\lambda^{-3}$ , whereby  $\lambda$  stands for the mean free spacing (STROEVEN, 1999; STROEVEN and STROEVEN, 2001b; HU *et al.*, 2006).

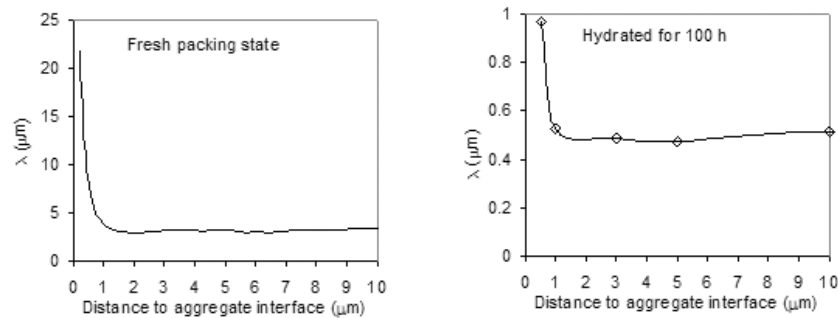


Fig. 12. Mean free spacing plotted against distance to the aggregate interface in the fresh packed model concrete with  $w/c = 0.3$  (water to cement ratio in weight terms), cement specific surface area of  $340 \text{ m}^2/\text{kg}$  (left), and in the hardened concrete hydrated for 100 hours (right).

The hydration algorithm in SPACE is described in the international literature, whereby the outward hydrating cement particles follow an almost similar description as in HYMOSTRUC3D (STROEVEN, 1999; STROEVEN and STROEVEN, 1997, 2001a). The more complicated situations arising from multiple-merging particles are elaborated for all practical cases (Fig. 13). The spherical particle is thereby replaced by a pentakis dodecahedron for efficiency reasons.

Very interesting and highly intriguing studies are performed on *concrete porosity* (HU, 2004; CHEN *et al.*, 2006). Connected, highly irregularly shaped pores build up a complex spatial network structure. Model cements of equal fineness lead to different total porosities despite mixed with the same amount of water when aggregate grain surfaces enclose the paste, or are more remote. This is simulated and illustrated in Fig. 14. At the center, a fully

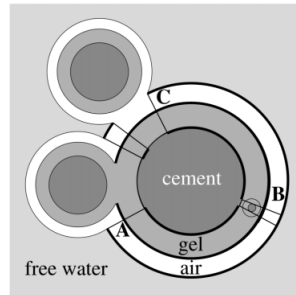


Fig. 13. Interaction of hydrating cement particles envisaged in the hydration algorithm.

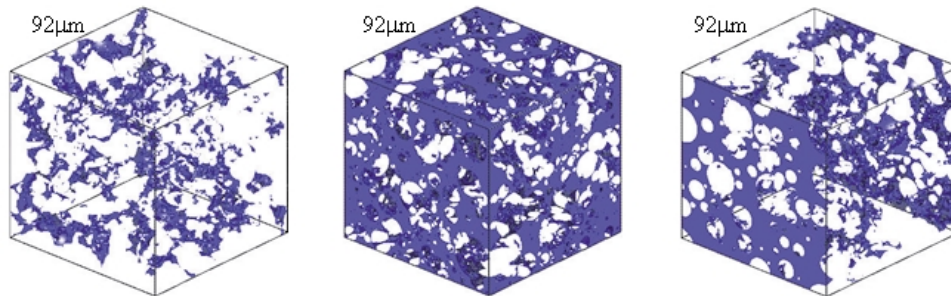


Fig. 14. Total porosity (blue colour represents pores in front and black colour represents pores in background) for different boundary conditions at ultimate degree of hydration (fineness  $300 \text{ m}^2/\text{kg}$ , water to cement ratio is 0.3) (CHEN *et al.*, 2006).

enclosed cement pocket is simulated; at the left, the aggregate surfaces are remote, so periodic boundaries are employed in the simulation. A mixed situation is shown at the right, whereby two parallel surfaces are rigid (aggregate grain surfaces) and the other four periodic (remote aggregate surfaces).

Total porosity is a global measure that has engineering relevance when pore space is uniformly distributed. Whether this is reflecting reality can readily be investigated. CHEN employed for this purpose SPACE-generated fresh cements that were hydrated by HYMOSTYRUC3D (basically, similar as in SPACE). This system encompasses facilities for 3D reconstruction by serial sectioning. Hence, total porosity and connected fraction of porosity were determined as function of the degree of hydration in cubical elements of diminishing size obtained from the original ones by successive removal of surface layers (Fig. 15). Total porosity and connected fraction of porosity are plotted at 75% of ultimate degree of hydration (UDH) for these cubical elements of reduced size in Fig. 16. Obviously, total porosity, and even stronger connected fraction of porosity, develops a gradient structure in the ITZ, with maximum value at the aggregate grain surfaces.

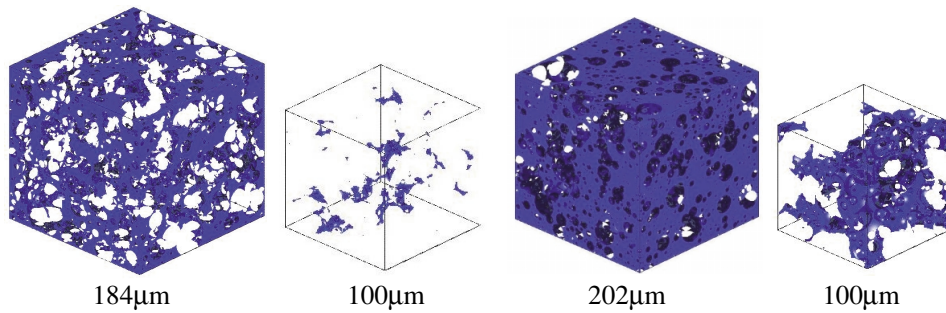


Fig. 15. Two cubes with rigid boundaries of fully hydrated cement pastes (left: UDH = 0.748; right: UDH = 0.991) based on different water to cement ratios (left:  $w/c = 0.30$ ; right:  $w/c = 0.50$ ). Additionally, central cubes are displayed that result from successive removal of all thin surface layers totaling ITZ thickness. Porosity differences are obvious (CHEN *et al.*, 2006). Color coding is as in Fig. 14.

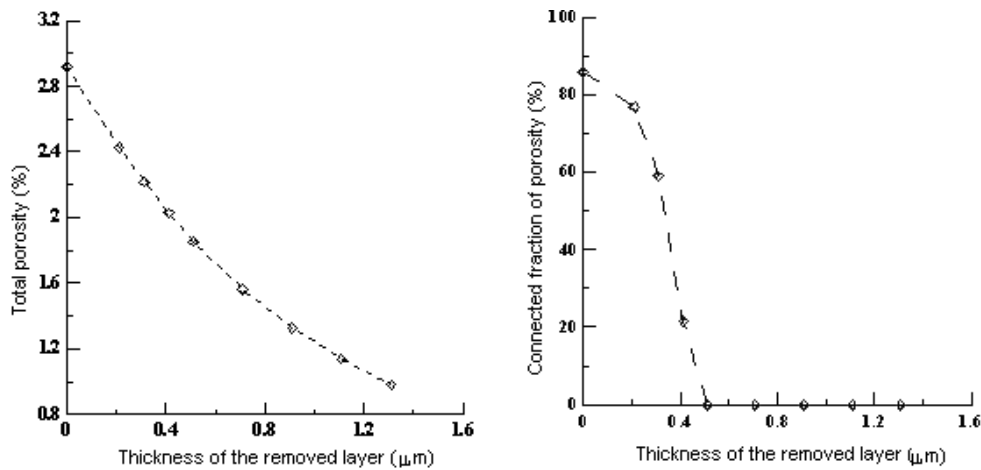


Fig. 16. Connected porosity is restricted to a narrower zone ( $0.5 \mu\text{m}$ ) in the ITZ of SPACE-generated compupaste ( $w/c = 0.3$ ; Specific surface area =  $300 \text{ m}^2/\text{kg}$ ) between aggregate grain surfaces (container walls) than total porosity (limited to zone of  $2 \mu\text{m}$ ) at about 75% DOH (CHEN *et al.*, 2006).

Of paramount engineering interest is the gradual decline in connected fraction of porosity during maturation. Reliable process information can only be provided by concurrent algorithm based systems, like SPACE. Figure 17 reveals major differences with results obtained on the same cement paste by the RSA-based HYMOSTRUC3D system. Configuration sensitivity declines during the process, so that the different de-percolation threshold values (porosity at which connected fraction is zero) at the intersection with the horizontal axis of the different systems are similar. Additional information is offered on the effect of the resolution of the approach. Obviously, the effect becomes negligible when the resolution is high enough.

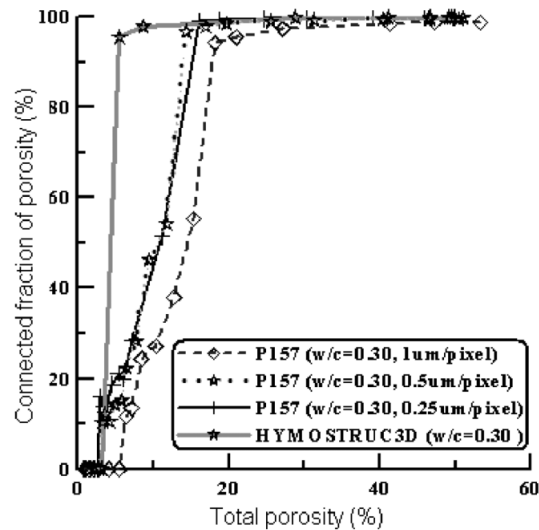


Fig. 17. Evolution of pore de-percolation during hydration as predicted by different computer simulation systems (CAS versus RSA);  $w/c = 0.3$  and Blaine fineness level is  $157 \text{ m}^2/\text{kg}$ .

## 6. Discussion and Conclusions

Modern computer facilities allow the development of concurrent algorithm-based discrete element simulation systems in the field of concrete technology that can produce concrete in virtual “reality” (*compucrete* on meso-level and *compupaste* on micro-level) as realistic representations of *realcrete*. This renders possible studying in economic and reliable way configuration-sensitive features of material structure that underlie structure-sensitive material properties. Major part of the aspects of material behaviour engineers are interested in is probably to some degree structure-sensitive. So, RSA systems should be selected only when proven leading to reliable results for the objected purpose.

## REFERENCES

- BALLANI, F. (2005) A case study: Modeling of self-flowing castables based on reconstructed 3D images, in *Proceedings of 9th Eur. Congr. Stereol. Image Anal.* (eds. J. Chraponski, J. Cwajna and L. Wojnar), pp. 282–288, Polish Soc. Stereol., Krakow.
- BENTZ, D. P., GARBOCZI, E. J. and STUTZMAN, P. E. (1993) Computer modeling of the interfacial transition zone in concrete, in *Interfaces in Cementitious Composites*, pp. 107–116, E&FN Spon, London.
- BREUGEL, K. VAN (1991) Simulation of hydration and formation of structure in hardening cement-based materials, Ph.D. Thesis, DUP, Delft.
- CHEN, H., STROEVEN, P., YE, G. and STROEVEN, M. (2006) Influence of boundary conditions on pore percolation in model cement paste, *Key Engr. Mat.*, 302–303, 486–492.
- DAI, D. D., HU, J. and STROEVEN, P. (2005) Particle size effect on the strength of rice husk ash blended gap-graded Portland cement concrete, *Cem. Concr. Comp.*, **27**, 357–366.

- DIEKÄMPER, R. (1984) *Technische Wissenschaftliche Mitteilungen der Inst. für Konstruktiven Ingenieursbau*, Ruhr Universität Bochum.
- GILKEY, H. J. (1950) The zig-zag course of concrete progress, *Journ. Americ. Concr. Inst.*, **21**, 8–18.
- HU, J. (2004) Porosity of concrete-morphological study of model concrete, Ph.D. Thesis, DUP, Delft.
- HU, J., STROEVEN, M. and STROEVEN, P. (2006) Exploitation of particle migration mechanisms to promote economy and ecology alike in concrete technology. *Key Engr. Mat.* **302**, 479–485.
- MEAKAWA, K., CHAUBE, R. and KISHI, T. (1999) *Modeling of Concrete Performance-Hydration, Micro-Structure Formation and Mass Transport*, E&FN Spon, London.
- ROELFSTRA, P. E. (1989) A numerical approach to investigate the properties of numerical concrete, Ph.D. Thesis, Lausanne, EPFL-Lausanne.
- RÖTHFUCHS, G. (1962) *Betonfibel, Band 1*, Bauverlag, Wiesbaden/Berlin.
- STROEVEN, M. (1999) Discrete numerical modelling of composite materials, Ph.D. Thesis, DUP, Delft.
- STROEVEN, M. and STROEVEN, P. (1996) Computer-simulated internal structure of materials, *Acta Stereol.*, **15**(3), 247–252.
- STROEVEN, M. and STROEVEN, P. (1997) Simulation of hydration and the formation of microstructure, in *Computational Plasticity*, pp. 981–987, CIMNE, Barcelona.
- STROEVEN, M. and STROEVEN, P. (1999) SPACE system for simulation of aggregated matter; application to cement hydration, *Cem. Concr. Res.*, **29**, 1299–1304.
- STROEVEN, P. (1973) Some aspects of the micro-mechanics of concrete, Ph.D. Thesis, DUT, Delft.
- STROEVEN, P. (1981) Methodological aspects of a study of particle and wire dispersion in cementitious materials, *Proc. 3rd Europ. Symp. Stereol.*, Ljubljana, *Stereol. Jugosl.*, **3**/Suppl. 1, 309–314.
- STROEVEN, P. and GUO, W. (1989) Structural modelling and mechanical behaviour of steel fibre reinforced concrete, in *Fibre Cements and Concretes, Recent Developments*, pp. 345–354, Elsevier Appl. Sc., London.
- STROEVEN, P. and STROEVEN, M. (2000) Assessment of particle packing characteristics at interfaces by SPACE system, *Image Anal. Stereol.*, **19**, 85–90.
- STROEVEN, P. and STROEVEN, M. (2001a) SPACE approach to concrete's space structure and its mechanical properties, *Heron*, **46**(4), 265–289.
- STROEVEN, P. and STROEVEN, M. (2001b) Reconstructions by SPACE of the interfacial transition zone, *Cem. Concr. Comp.*, **23**, 189–200.
- STROEVEN, P., GUO, Z., HE, H., HU, J. and STROEVEN, M. (2007) The making of realistic computer generated concrete, *Journ. Americ. Soc. Test. Mat. Int.* (submitted).
- WILLIAMS, S. R. and PHILIPSE, A. P. (2003) Random packings of spheres and spherocylinders simulated by mechanical contraction, *Phys. Rev.*, **E67**, 051301, 1–9.
- ZAITSEV, J. W. and WITTMANN, F. H. (1977) Crack propagation in a two-phase material such as concrete, in *Fracture 1977*, Vol. 3, ICF4, pp. 1197–1203, Waterloo (Ca).