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On the usefulness of discrete element computer modeling of particle packing for material characterization in concrete technology

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Abstract. Discrete element modeling (DEM) in concrete technology is concerned with design and use of models that constitute a schematization of reality with operational potentials. This paper discusses the material science principles governing the design of DEM systems and evaluates the consequences for their operational potentials. It surveys the two families in *physical discrete element modeling* in concrete technology, only touching upon probabilistic DEM concepts as alternatives. Many common DEM systems are based on random sequential addition (RSA) procedures; their operational potentials are limited to low configuration-sensitivity features of material structure, underlying material performance characteristics of low structure-sensitivity. The second family of DEM systems employs concurrent algorithms, involving particle interaction mechanisms. *Static* and *dynamic* solutions are realized to solve particle overlap. This second family offers a far more realistic schematization of reality as to particle configuration. The operational potentials of this family involve valid approaches to structure-sensitive mechanical or durability properties. Illustrative 2D examples of fresh cement particle packing and pore formation during maturation are elaborated to demonstrate this. Mainstream fields of present day and expected application of DEM are sketched. Violation of the scientific knowledge of to day underlying these operational potentials will give rise to unreliable solutions.

Keywords: concrete; concurrent-algorithm; dispersion; microstructure; discrete element modeling.

1. Introduction

DEM is a scientific sub-discipline pursuing a schematization of reality with operational potentials. This is a very compact description. It says that the real world is represented by a model; in the present case a virtual one. Hereby, "model" stands for "a schematic description of a system, theory or phenomenon that accounts for its known or inferred properties and may be used for further study of its characteristics" (Wikipedia). Or stated in a more popular way by Maier at a conference paper presentation (Maier *et al.* 2005), a "model is a heroic simplification in order to grip the essentials." Where the given definition speaks of "it may be used for", reference is given to the *model's potential usefulness when operated or exploited for proper tasks*.

Searching by Google offers about 357,000 references to "DEM", evidencing the successful development the last quarter of a century of many discrete element models in virtual reality, thereby making use of modern computer facilities. An extensive review of DEM and its industrial

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applications by Tüzün & Cleary (2007) gives a survey of the different approaches of to day, not mentioning a single sequential random addition system (RSA). A PhD study focusing on DEM by O'Connor (1996) explicitly deals with spatial sorting and contact detection algorithms that are relevant for concurrent systems. So, although in the scientific community RSA systems seem outdated, they are widely applied in concrete technology, the field on which this paper will focus. Therefore, this paper employs such a system (for which Delft-made HYMOSTRUC3D is considered a representative example) in comparison with a concurrent one based on commonly used Newtonian particle mechanics for assessment of particle dispersion (Tüzün & Cleary 2007, Stroeven 1999), for which Delft-made SPACE/HADES system is seen as representative example. Moreover, it is felt that the Newtonian process simulates the compaction by vibration production conditions of cementitious materials, so can be considered a proper schematization of reality in concrete technology. O'Connor (1996) summarizes the various methods in vogue (around 1995) by giving three overall characteristics, namely

- they are predominantly based on spheres and discs;
- they are using up to thousands of objects;
- they are in many cases of 2D nature.

In that sense, the Delft-made concurrent algorithm-based DEM system SPACE (developed around the same time) may be seen as quite advanced. The even more advanced HADES system (based on similar Newtonian mechanics for particle dispersion) was developed in the present century. The aforementioned comparison will allow demonstrating "operational potentials" to be fundamentally different between the two approaches. From Tüzün and Cleary (2006) it becomes clear that most of the available DEM systems were developed to execute specific tasks for which verifications may have been executed. However, using them in other fields would require investigating the similarity between actual group characteristics (the real world) and the simulated ones. So, the principles outlined in this paper should be applied.

Virtual modelers in the field of cement-based materials like concrete have been associated with alchemists, although fortunately in a metaphoric sense (van Breugel 2004). Alchemy has always had a flavor of continual, senseless quests for producing gold in obscure settings; and many followed this quest throughout history, indeed unsuccessfully. As an example, at the end of the 18th century, Hennig Brand took soldiers' urine for this purpose. His hope for success probably came from the color resemblance, but he did not rely on an objective, cognitive strategy based on the *scientific knowledge of that day*. He did not produce gold-but serendipity worked for him: he was the first to synthesize phosphorus that was in the urine, although he is not generally recognized for this achievement (Bryson 2004). So, what can be said in that regard about modeling the structure of cementitious materials by DEM? And, in a wider perspective, how does this sub-discipline fare within the field of concrete technology? For sure, alchemy is still around us, whenever and wherever modern scientific knowledge of to-day is not properly applied. This is probably in large part the result of pressure to come up with practical concepts that are as simple as possible. The following two examples illustrate this.

1) The elastic constants (such as Poisson's ratio and Young's modulus) of a composite material like concrete have been formulated in an optimum way (*i.e.*, solely based on composition) by the upper and lower bounds proposed by Hashin and Shtrikman (1963). Their derivation is based on scientific principles, even of to-day. Since the gap between the bounds can be significant, Paul (1960) proposed to take the arithmetic average as the *best estimate* for the elastic constants. This is "alchemy". This average is not necessarily closer to the real value than either one of the bounds.

Additional geometric parameters of material structure would be necessary to narrow the distance between the bounds in a scientific approach.

2) The second example concerns fiber reinforcement efficiency in concrete. The number of fibers reinforcing a crack is obviously a leading parameter. But the orientation of such fibers should have influence, too. In a thin sheet, the orientation distribution of fibers *in bulk* (which is fundamentally different from those reinforcing the crack) might be assumed 2D-like. Distribution in a bulky element could be assumed 3D (formally, isotropic uniformly random: IUR). Again this does not hold for the reinforcing fibers—a problem generally overlooked, as in the 2D case. However, to assume the real fiber distribution in an element with arbitrary section dimensions closest to the arithmetic average of the 2D and 3D fiber distributions is "alchemy", although indeed offering a practical and as-simple-as-possible solution. Still, the scientific knowledge of to-day allows one to do better, *i.e.* using gradient structures theory (Stroeven and Hu 2006).

The foregoing illustrates that systematically exploring new territories (such as the complicated material structure in virtual reality), provided this is based on "modern, scientific methodology", is alien to alchemy. It can only be associated with alchemy when researchers make use of outdated knowledge and fall back, so to say, on alchemist-like approaches. Hence, when "looking for gold"-also in modeling efforts-is pursued in a non-scientific framework, the association with alchemy can be justified, and not just in a metaphoric sense. The end products of the science-based modeling approaches can be hypothesized. The research strategy that will lead the researcher to his hypothesized end product is a cognitive and not an affective one, thus leaving no room for the "hope for finding gold." Still, an alchemy-like approach can incidentally lead to unexpected success; this is the *serendipity* dimension in research.

This paper aims discussing the relevant principles of modern scientific knowledge of to-day. This will ultimately allow considering the conditions to which the alchemy connotation could apply. The hypothesis that will be discussed in this paper is that alchemy is excluded *when the model's potential usefulness is operated or exploited for proper tasks.* Hence, we will not survey the many different approaches in vogue in concrete technology; neither will we discuss their pros and cons in the light of the modern scientific knowledge of to day. Nevertheless, relevant concurrent algorithm strategies to solve the particle interaction problem are mentioned. The scientific basis that is provided in this paper would allow evaluating the operational potentials, or the proper tasks that can be performed by specific DEM systems, considering the algorithms on which particle dispersion is relying. This is a task for those exploiting the various systems, so that reliability of obtained information could be guaranteed for the users. This is accomplished in an illustrative way for representative systems of the two major families of DEM in concrete technology.

2. Materials science principles

Cementitious materials belong to the category of macroscopically heterogeneous particulate composites. To appreciate this statement, a closer look is required at the concept of stochastic heterogeneity for particulate materials (Stroeven *et al.* 2008). *Stochastic heterogeneity* is associated with the scatter in data of the same descriptive parameter pertaining to a series of identical samples (specimens or images). Hence, changing linear dimensions of specimen or image would imply heterogeneity to change; it is obviously not a material parameter. Recording another parameter from the same sample would also lead to a modified scatter level (*i.e.*, heterogeneity), of course.

Upon increasing linear dimensions of samples, heterogeneity will finally be reduced to an acceptable low level, which is denoted *homogeneity*. It is achieved for the Representative Volume Element (RVE) when dealing with specimens, and for the Representative Area Element (RAE) when analyzing images. So, basically, specific RVE and RAE sizes can be defined for each descriptive parameter of material structure or of material behavior. The direct implication is that on images of identical size, heterogeneity of different descriptive parameters will be different in a sub-RAE (*i.e.,* smaller than RAE) sampling design. The same can be stated about different descriptive parameters (*e.g.*, LOP versus fracture energy) in a sub-RVE testing approach. The consequences of this will be made clear in what follows.

Naturally, aspects of material (mechanical or durability) performance will rely on various characteristics of material structure. On the one hand, material structure can be defined by "how much" of the relevant material component is at issue. This is associated with volume fraction or volume-weighted particle density in a particulate material. Mass is a material property solely depending on volume fractions of material components. The material feature is defined as a *configuration-insensitive* or *composition parameter*, the material property as a *structure-insensitive* one (Stroeven 1973, Freudenthal 1950, Holliday 1966). A configuration-sensitive parameter provides information on the so-called group effect, *i.e.,* on size, shape, and spacing of the particles forming the group. Different descriptive parameters of material structure (*e.g.,* surface-to-surface spacing versus mean free spacing of particles) will be to different degrees sensitive to particle configuration. The same can be said about aspects of material performance. Whereas the deformation or load at the first crack will be highly sensitive to details of material structure, Young's modulus will not; the first property is therefore denoted as structure-sensitive. It is a small step seeing that the RVE for a highly structure-sensitive property can exceed the one for a structure-insensitive one to a considerable degree (Stroeven 1973, Stroeven and Stroeven 2001a, Stroeven *et al.* 2008). These fundamental materials science concepts are not new, but can be found in relevant text books. According to Freudenthal (1950), "it should be noted that if there are n independent geometrical parameters (such as concentration, particle size, orientation, etc.), there will be n values for the representative cells since each geometrical parameter has an independent scale of homogeneity...To put this another way, heterogeneity cannot be uniquely described by a single geometrical variable"

Descriptive parameters with configuration-sensitive character (in quantitative image analysis approaches), or of structure-sensitive nature (in testing approaches using 3D specimens) lead to negatively skewed probability density functions, like in the classical case of Weibull's approach to brittle strength (Stroeven 2003, Epstein 1948). The latter is directly linked up with the well-known size effects in fracture mechanical testing. The parameters defining such curves (like mode value and scatter/heterogeneity) change their values when image or specimen sizes are modified, unless one makes use of representative elements, which is more the exception than the rule in concrete

Table 1. Average spacing parameters pertaining to nearest surface-to-surface spacing of a continuously-graded mixture of 5 to 10 mm aggregate grains molded in containers with periodic boundaries of different sizes (all measures in mm). For more information, see Chen *et al.* (2006).

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

technology. These effects are depending on the degree of configuration- or structure-sensitivity, for given size of image or specimen on which investigations are based. Nearest neighbor (NN) distribution curves for the aggregate grains of the same model concrete, however produced in containers of different sizes, reveal such shifts in average values, as demonstrated by Table 1. Hence, the degree of bias introduced in sub-representative designs is unknown, unless assessment is possible on the basis of experimental data.

3. DEM's mainstream approaches in concrete technology

The materials science concepts described in the foregoing have direct impact on experimental research (either testing specimens, or quantitatively analyzing images) (Stroeven 2003, 2005, Stroeven *et al.* 2008). But they are also of paramount importance for modeling on the basis of the *scientific knowledge of to-day*. This can easily be seen. When interested in estimating Young's modulus of a particulate material, reality can be schematized more "crudely" than when interested in the crack initiation strength of a specimen subjected to shrinkage. In the first case, we deal with a property of low structure-sensitivity. Major parameters are the volume fractions of the composing parts. Hence, basic modeling requirement is that the particulate model should just contain the same amounts of composing components. Disparities with reality in size distribution and in particle dispersion are of lower relevance. What is more, the simulated element can be of sub-RVE size, since the probability density functions of mass, and approximately also of Young's modulus will be Gaussian (Stroeven 1973, Stroeven *et al.* 2008). Hence, *schematization of reality with operational potentials* is *not very demanding* in this case. All random generator-based discrete element computer simulation systems developed the last quarter of a century in concrete technology (van Breugel 1991, Roelfstra 1989, Diekkämper 1984, Bentz *et al.* 1993, Meakawa *et al.* 1999) will suffice. Roelfstra (1989) demonstrated convincingly that even a 2D version of such approaches could provide unbiased estimates when dealing with structure-insensitive aspects of material behavior, like permeability.

The *schematization of reality with operational potentials* is quite demanding, however, when the researcher's interest is in properties that are structure-sensitive. The schematization of reality should be more sophisticated in such cases, because configuration of particles, the so-called group effect, will influence these properties. Moreover, sub-RVE designs in computer simulation will lead to biased results, because of the skewness of the probability density function for the structure-sensitive property at issue, such as of the earlier mentioned brittle strength (Stroeven 2003). This is known for a long time, as expressed by Epstein (1948): "Many scientists accept the fact that the Gaussian distribution plays a fundamental role in science and, in fact, there are many who feel that this is the only distribution which nature calls truly her own … however, in a certain class of phenomena the characteristic distributions are far from normal and are, in fact, strongly skewed to the left".

DEM systems nowadays in vogue in concrete technology for forming granular packing of hard particles can be placed, therefore, in two distinctive groups. The first group, based on so-called *concurrent algorithms*, involves the densification of a fixed number of particles. The second group, based on *sequential algorithms*, involves progressively adding more particles to a fixed volume (Hu and Stroeven 2005, Williams and Philipse 2003). Significant part of popular computer simulation approaches in concrete technology fall in this second category. They generate granular packing of spheres or particles with other idealized shapes by *random sequential addition*, RSA. These two

systems will be extensively compared in what follows.

So far it is taken for granted that physical discrete element modeling would be the only way to "schematizing reality". It certainly is the most intuitive approach, and received therefore prime attention in concrete technology. Reference should be given, however, to probabilistic discrete element models as a schematization of reality with operational potentials. Once such a model is found to properly represent reality (seeing the fundamental relationship between type and degree of schematization and degree of structure sensitivity of the objected property), the characteristics of the model are known. This is not the case with physical discrete element simulation. All probabilistic models start from a Poisson process that is also at the basis of most physical modeling approaches. A distinction is made between tessellations and poly-phased models. In the first category are Voronoi and Poisson tessellations, and the Johnson-Mehl model; all sub-divide (2D or 3D) space. The poly-phased models encompass Boolean and dead-leaves models, among many others. This paper not intends to go into any detail of such approaches. Two active "schools" can be mentioned, *i.e.*, the "Centre Morphologique et Mathematique" in Fontainebleau (Fr), and the "Bergakademie Freiberg", (Ger), claiming such probabilistic models potentially (even) more promising than the physical ones (Dequiedt *et al.* 2001, Ballani 2005, Bezrukov *et al.* 2001).

4. Concurrent versus sequential models

For the present paper we have therefore reduced the scope to comparing in more detail concurrent and random sequential modeling concepts. The schematization of reality will be different in the two cases, although the simulation of a packed particle assembly in a container can start in both cases from a Poisson field of points. To gauge an idea of the efforts involved in the next stage of the simulation process, volume fractions of 50 to 75% have to be realized for aggregate or cement paste in the fresh state at low water to cement ratios. The problems that should be emphasized are qualitatively visualized by means of the 2D set up of Fig. 1. Already at this low area fraction, "particles" do overlap. This problem increases disproportionately at higher area fractions. The two concepts employ different strategies to tackle this fundamental problem.

Particles are placed in the sequential system from large to small on the preconceived Poisson field positions (for relevant equation, see *e.g.*, Ougouag *et al.* 2006) of which part cannot be exploited, however, due to insufficient spacing, as revealed by Fig. 1. The consequence is that new positions are randomly assigned to remaining particles until overlap is avoided. This is a time-consuming process since the number of re-generations dramatically increases when 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 of the cases the production of computer concrete with 40% spherical aggregate failed. Moreover, the re-generation process replaces near-contact situations, as shown in Fig. 1, by "on average" more uniform dispersions. RSA systems, as a consequence, poorly reflect a natural phenomenon in particulate matter like particle grouping, heaping or clustering as shown in Fig. 2 for aggregate and reflected by Fig. 3 for pore structure. According to Williams and Philipse (2003) is therefore "any relation between these RSA packings and an experimental granular packing at best tenuous." As a consequence is concrete's patch structure (Diamond and Thaulow 2006) also less pronounced, and is pore de-percolation during maturation delayed, as will be demonstrated later.

The strategy to solve the overlap problem in concurrent algorithm-based systems is either of static

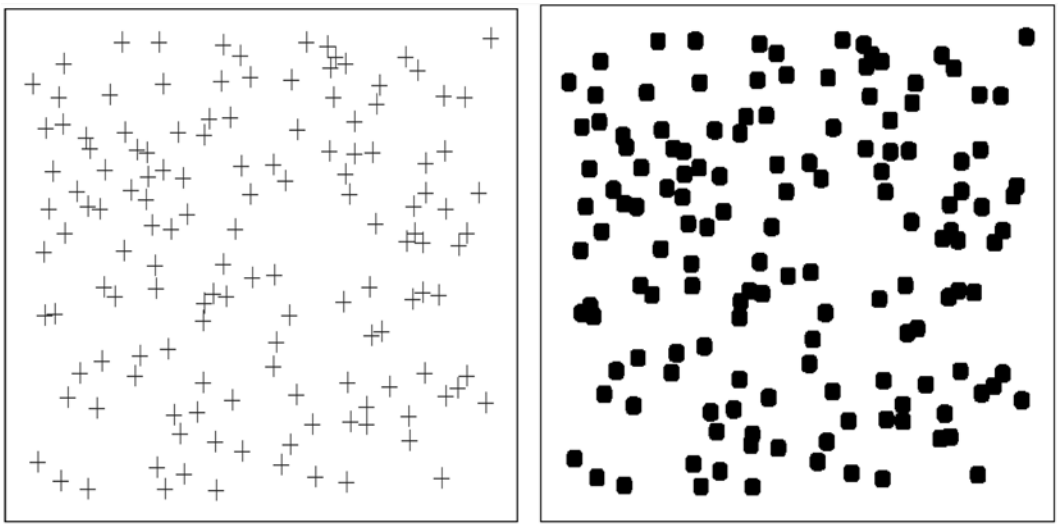

Fig. 1. Random 2-D distribution of points (left) on which mono-size "particles" are positioned with 13% coverage of area whereby overlap is obvious (right).

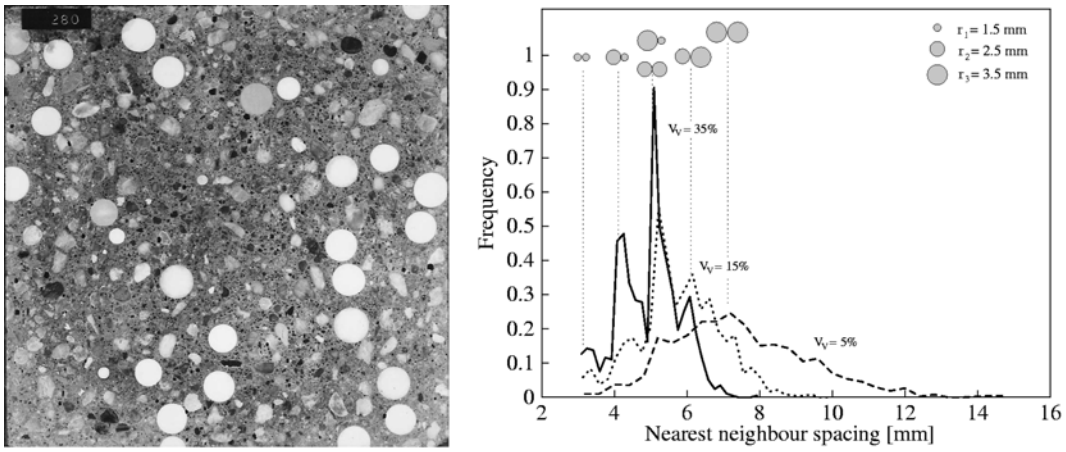

Fig. 2. Section of concrete cube (left) reveals clustering tendency among grains in largest aggregate fraction of 16 mm mono-size ceramic spheres (9.2% by volume) (Stroeven 1973). The nearest neighbor distance distributions for SPACE-generated model 'concretes' containing three aggregate grain sizes (r stands for grain radius) show increasing clustering at higher volume fractions of aggregate (Stroeven and Stroeven 2000).

or of dynamic nature. In both cases, the container size can be initially enlarged so that all particles can be positioned at Poisson points, or otherwise. Thereupon, the container size is gradually reduced and the grain system squashed. Mechanical contraction (Williams and Philipse 2003) is a *static solution* that involves local shifting of particle positions to eliminate overlap. This system is also developed for sphero-cylinders up to an aspect ratio of 160 (simulating fiber reinforcement). Jammed states are found for spheres at 63.1% and for sphero-cylinders with an aspect ratio of 0.4 at 69.5%. The SPACE system, developed at Delft University of Technology, realizes compaction by a *dynamic algorithm*, which is also supposed to imitate the *production stage* of the material. The

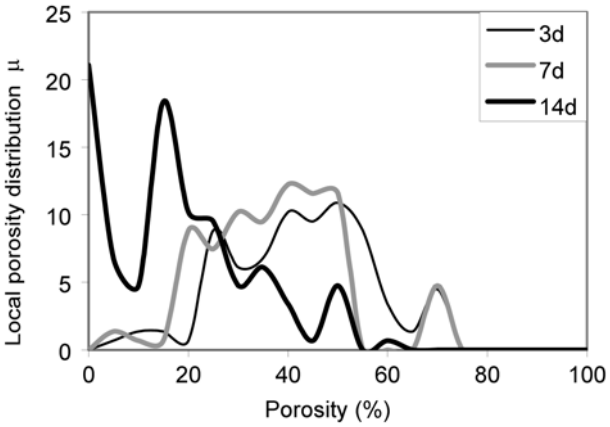

Fig. 3. Local porosity distributions μ for cement paste with w/c=0.6 at 3, 7 and 10 days of hydration, respectively. Field size is 19 μm (Hu and Stroeven 2005). Results reveal the non-uniform (or patchy) distribution of the pores in the cement paste. Samples were prepared by Ye (2003). The 40×40×160 mm prisms were de-molded after 1 day and cured at 20°C and 90%RH. After vacuum-drying, they were impregnated by low-viscosity epoxy, cut and sections polished (Hu 2004).

forces added to the particles can be manipulated, so that "sticky" particle contacts (or particle repulsion) during the production of the model material (*i.e.*, fresh cement paste) can be simulated. Also gravity effects can simply be included. The system contains a parameter for energy loss due to internal friction that can be used to consider differences in workability. 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 1996; 2000; 2001b). SPACE is based on hard spherical particles only. However, a new SPACE-like system has been recently developed allowing the use of soft arbitrarily shaped particles (the so-called HADES system (Stroeven *et al.* 2006)). This is to account for particle shape effects that seem to have more serious impact on packing than so far assumed in concrete technology. Also experiments where a granular mixture is subjected to external forces can be executed.

A wide range of other concurrent algorithms either static or dynamic are developed and employed in specific problem areas (Mościński *et al.* 1989, Markausas and Kačianauskas 2006, Tsunekawa and Iwashita 2001, O'Connor *et al.* 1997, Jodrey and Tory 1981, Ansell and Dickinson 1986, Li *et al.* 2006, Klosek 1997, Puri and Uomoto 2002). Specific mention is made of compaction of a model granular mix, whereupon successive shifting of particle positions and reduction of grain size is employed to eliminate particle overlap (Mościński *et al.* 1989), or the mixtures are just compacted by different means to get densest packing (Markausas and Kačianauskas 2006, Tsunekawa and Iwashita 2001). Next, a container is filled by successively dropping particles in the gravitational field (O'Connor *et al.* 1997, Jodrey and Tory 1981), an operation also performed by SPACE, *e.g.*, to simulate silo discharges (Fig. 4). Tüzün and Cleary (2007, pp. 22, 31, 32) present also information on this phenomenon. Maximum density is lower than obtained by other systems, and gradients may occur. Finally, Brownian movement and container size reduction have been applied to obtain dense packing state of particles (Ansell and Dickinson 1986, Li *et al.* 2006). The present authors like to make special reference to major DEM contributions to concrete technology in the USA by the cooperation efforts of Sandia National Laboratories and MIT (*e.g.*, www.nwer.sandia.gov/wlp/factsheets/dem.pdf), and, particularly, by the numerous papers of Garboczi, Bentz, and coworkers at

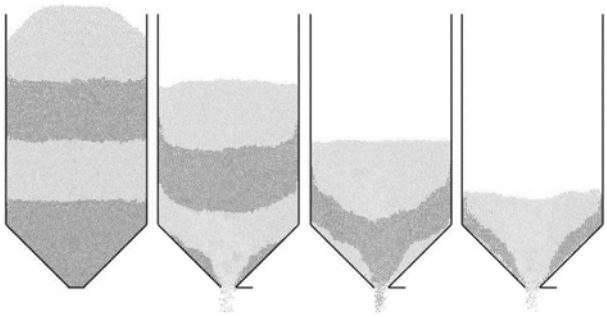

Fig. 4. Silo filled by multi-sized grains during discharge, simulated by HADES. Layers are color-coded to assess discharge mechanisms as a function of mix characteristics (particle size distribution, particle shape) and silo properties (smoothness of internal surfaces, size ratio of particles and opening). For similar type of simulations, see Tüzün and Cleary (2007).

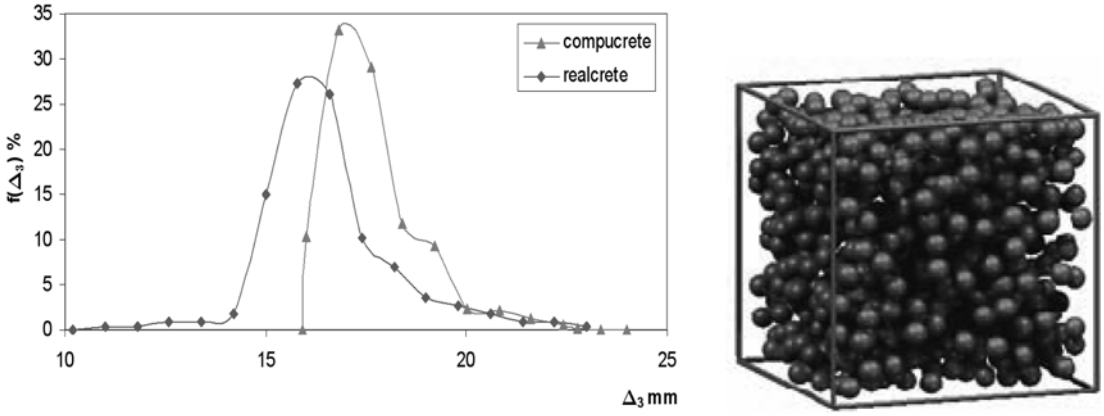

Fig. 5 (left). Spatial frequency distribution of the nearest neighbor distance, Δ_3, in realcrete (example in Fig. 2) and compucrete (Fig. 5 at the right), both containing 20.6% by volume of 16mm mono size spherical aggregate. Experiments encompassed 250 mm cubes of which 25 mm was removed on all sides. Assessment of the nearest neighbor distance was accomplished after serial sectioning and 3D reconstruction (Stroeven 1973; Stroeven 2008). The differences are particularly due to the relatively low sensitivity of the experimental approach.

NIST ("Google" offers 17.800 references to "Garboczi Bentz").

At the jammed state, particle densities between 72% and 75% have been obtained by SPACE, depending on the size distribution function, which were found in very good agreement with experimental observations on aggregate density (Stroeven *et al.* 2006, Stroeven and Stroeven 1999). Comparison of gradient characteristics of mono-size particles packed in a container with rigid boundaries to a volume density of 0.62 with experimental data of Shinohara (1984) demonstrated precisely the same long-range fluctuating behavior. At a lower particle density (0.32) this long-range fluctuations were still found, although less pronounced. They were completely lacking however in a simulation by SRA system (Stroeven 1999). Comparison of the 3D distribution of the nearest neighbor center-to-center distance (Δ_3) in experiments and SPACE simulated concrete resulted also in satisfactory agreement in this tough configuration test (Fig. 5).

The hydration algorithm in SPACE is described in the international literature, whereby the outward

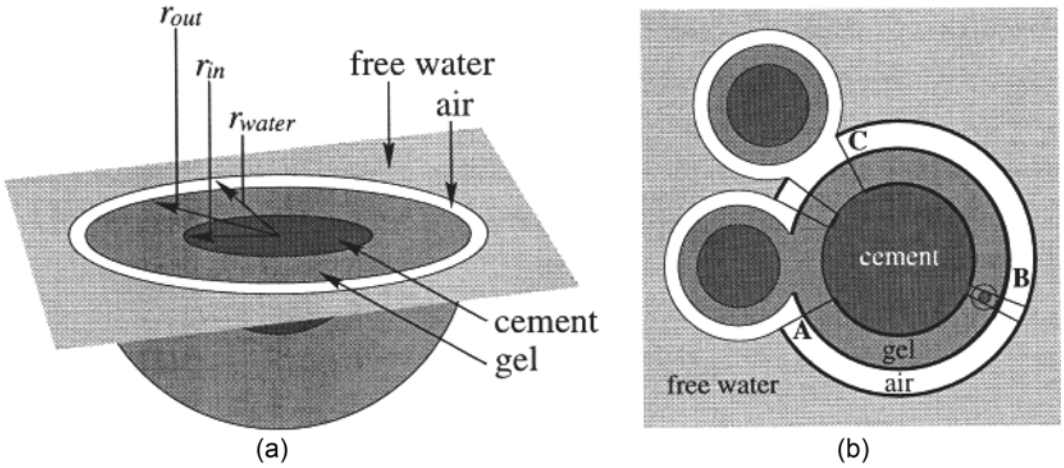

Fig. 6(a) Geometrical representation of hydrated cement and (b) various contact situations between cement particles (according to Stroeven 1999).

growing cement particles follow almost similar description as in RSA-based HYMOSTRUC3D. The more complicated situations arising from multiple-merging particles are elaborated for all practical cases that can arise (Fig. 6). The spherical particle is thereby replaced by a pentakisdodecahedron for efficiency reasons. This hydration algorithm allows studying matured cementitious composites (Stroeven *et al.* 2006, Stroeven and Stroeven 1996, 1997, 2000, 2001b, Stroeven 1999).

Simulations can be realized in containers with periodic or rigid boundary conditions. By inserting a flat rigid surface halfway in a container with periodic boundaries, also mixed situations can be simulated. This approach is followed in both types of DEM approaches. Basically, rigid surfaces allow the study of gradient structures in aggregate packing near the mould, or in size segregation of cement particle packing and in porosity in the Interfacial Transition Zone (ITZ) around aggregate particles. Prerequisite is however a proper dynamic concurrent algorithm for simulating size segregation in the ITZ, as realized in SPACE/HADES. Size segregation in the ITZ is of a long-range character, as stipulated earlier. In addition to the normal "wall effect", compaction by vibration stimulates size segregation due to the Brazil Nut Effect (Stroeven *et al.* 2007). To be able simulating this long-range phenomenon, particles should be able moving over relatively long distance (say, 5 times their diameter) in the simulation set up. This can be realized by the Newtonian mechanism in SPACE/HADES. Static concurrent systems will fall short in doing this. The static concurrent system developed at the University of Utrecht (Williams and Philipse 2003) can realize packing densities of 63.1% for mono-size spheres and 69.5% for slightly non-spherical grains (*i.e.*, sphero-cylinders with aspect ratio of 0.4), revealing the significant effect of slight deviations in sphericity on packing. These packing densities are lower than can be achieved by SPACE. Moreover, application of random particle shifts after overlap detection in static concurrent systems will inevitably promote "randomness" in the resulting particle dispersion. So, when realistic particle spacing is required, this may lead to biases.

As stated earlier: modeling pursues a schematization of reality with operational potentials, which points to the *intimate relationship between the type and degree of schematization and the objectives for exploiting the operational potentials*. Not all aspects of the inherently complex system that concrete is have to be "realistically" schematized, but only those relevant for obtaining the unbiased

3D structure information on which the aspect of material performance relies the researcher is interested in. A complicated task, anyhow. Some of our questions will deal with aspects of material performance that have a low structure-sensitive nature. Using an RSA-based system would suffice in this case. Unfortunately, most problems of engineering relevance are definitely of structure-sensitive nature. A concurrent system should be employed in such cases.

The following example can be instrumental in understanding the above statement on degree of schematization versus operational potentials (*i.e.*, usefulness for the task). The total degree of hydration is a *global* measure for strength development, or self-healing capacity, at least to a certain maturation stage. In real concrete (*realcrete*) and simulated concrete alike, water moves to places it is needed. This may occur relatively easy in the RSA-based *compu(ter)crete* of which the cement particles are more evenly distributed than will occur in reality. Real cement particle dispersion will reveal particle clustering as a natural phenomenon. Free water movement to and from more isolated pockets will start stagnating at a less advanced stage of maturation due to particle clustering in realcrete and compucrete as simulated by concurrent systems. This affects the degree of hydration. Fortunately, *total* degree of hydration is probably quite structure-insensitive, so putting a low demand on the schematization of reality. Any particulate simulation system can do the job, because the actual dispersion of the particles has no major influence. On the other hand, a *similarity in total degree of hydration between experiments and simulation cannot be interpreted in terms of a similitude in particle configuration, of course.*

5. Illustrative 2D example of RSA versus concurrent simulation

Fig. 7 presents simple 2D "particle" structures cast in 50 μm containers of fresh cement paste with an area fraction of 0.4 consisting of spherical cement particles of 1 to 10 μm. The structure at the left is realized by SPACE, the one at the right by an RSA algorithm; the only difference is the spatial distribution of the particles. This allows demonstrating *the impact of configuration biases on structural descriptors*. Fruitful use of modern mathematical morphology methods can additionally

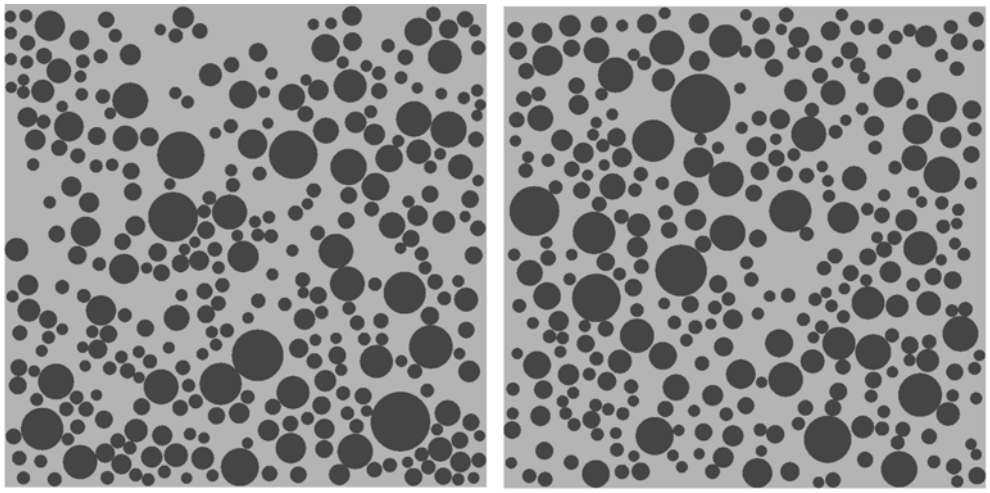

Fig. 7. Two-dimensional "particle" packing patterns simulated by dynamic mixing (left) and by RSA procedure (right) for 40% area coverage. This is employed as the fresh cement paste stage in Fig. 9.

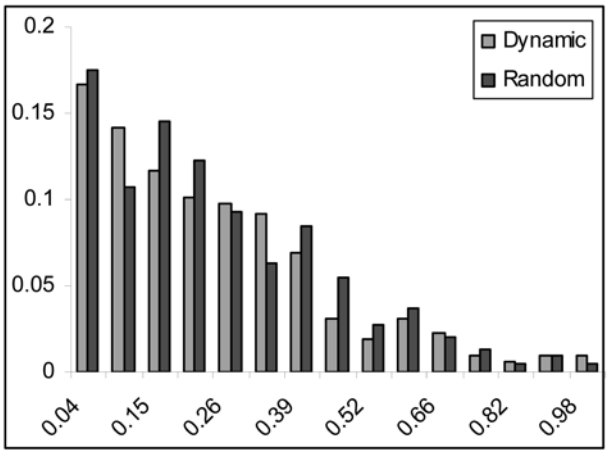

Fig. 8. Probability density of the 2-D surface-to-surface nearest neighbor distance, NND (as bar diagrams) for packing structures generated by concurrent (dynamic) and RSA (random) algorithms as shown in Fig. 7.

be demonstrated, despite the model's simplicity. Particle dispersion is (slightly) more uniform in the RSA pattern, as argued before. This structure is denoted as *random* in what follows.

The distribution probabilities (Fig. 8: histograms in 15 classes) of the so-called 2D surface-to-surface nearest neighbor distance (NND) are used to characterize the dispersion (configuration) of the particles. Mode value of the skew NND function is 0.04 μm for the SPACE structure, in agreement with Kendall and Moran (1963). Mean values of NNDs are 0.236 (left) and 0.262 μm (right) for the patterns in Fig. 7. Even in this relatively dilute *two-dimensional* system, the total number of contacts between particles is 8 for the SPACE structure, and zero in the random case. Differences can be expected much more dramatic when based on dense 3D grain packing.

When interested in the assessment of porosity in cementitious materials, RSA systems might suffice. However, when the focus is on the mutual arrangement of pores (*e.g.*, because of pore connectivity), concurrent algorithm-based systems should be employed to provide a reliable basis for progress. Particularly, correct information on *pore topology* requires realistic modeling of particle configuration in the fresh state that is underlying the hydration simulation. For illustration purposes, the two fresh 2D packing structures of cement particles (Fig. 7) are 'hydrated' by means of mathematical morphology operations (*i.e.*, dilation). After continuous dilation by a structuring element of 1-pixel (0.058 μm), the cement pastes are converted into binary images (Fig. 9), leaving the solid phase in white (cement particles and hydration products) and the pore space in black. Porosity is slightly higher in the dynamic structure (25.4 and 22.9%), indicating that the cement particles in the fresh state are clustering to a higher degree (as visualized by Fig. 7). Hence, even porosity is not a purely configuration-insensitive property!

The pore structures in Fig. 9 are quantitatively characterized by opening distribution, which has been demonstrated to provide reliable information on 3D pore size distribution and critical pore size (Hu 2004, Delfiner 1971). Fig. 10 plots the cumulative porosity distribution and pore size distribution functions for the pore structures in Fig. 9. It is interesting to see that the pore structure in the 'dynamic' cement has two dominating peaks at 0.92 and 1.55 μm, whereas in the 'random' cement the two peaks appear at 1.09 and 1.61 μm, respectively. These peaks are corresponding to the inflection points of the cumulative porosity distribution curves (Fig. 10 left) and are generally

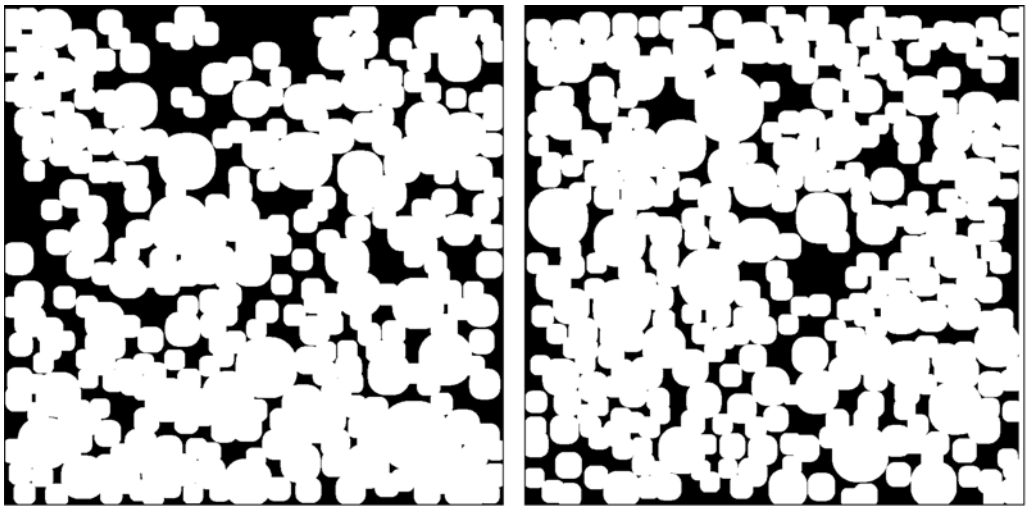

Fig. 9. Simulated 2D pore structure in the hydrated cements (fresh states shown in Fig. 7). Solid phase is indicated in white and pores in black.

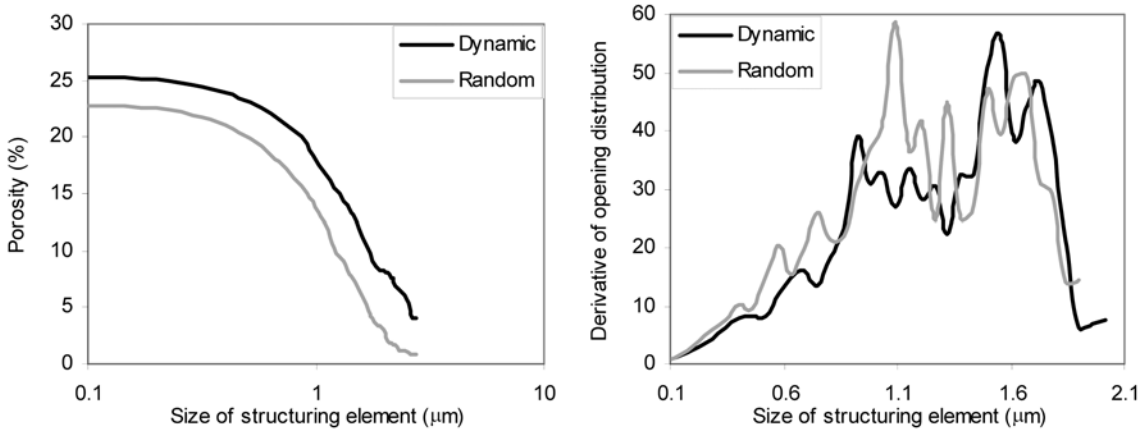

Fig. 10. Cumulative porosity distribution (left) and pore size distribution (right pertaining to Fig. 9

related to de-percolation threshold of pore space in cement pastes (Katz and Thompson 1986). This implies that, although the total porosity in the 'dynamic' cement is slightly higher, the pore structure is easier to de-percolate, therefore, the porosity connectivity is expected to be lower than in the 'random' cement at the same hydration stage. Fig. 12 shows the skeleton of the pore space in Fig. 10, composed of locally connected pore channels and isolated pores. It should be noted that this 2D simulation does not reflect the actual 3D situation; however, structure information of the simulated pore space sheds some insight on the influences of cement particle dispersion in the fresh state on the pore topology in the hydrated cement paste. The total skeleton lengths are 667 and 700 μm, corresponding to lengths per unit area (L_A) of 0.28 and 0.30 μm^{-1}, respectively.

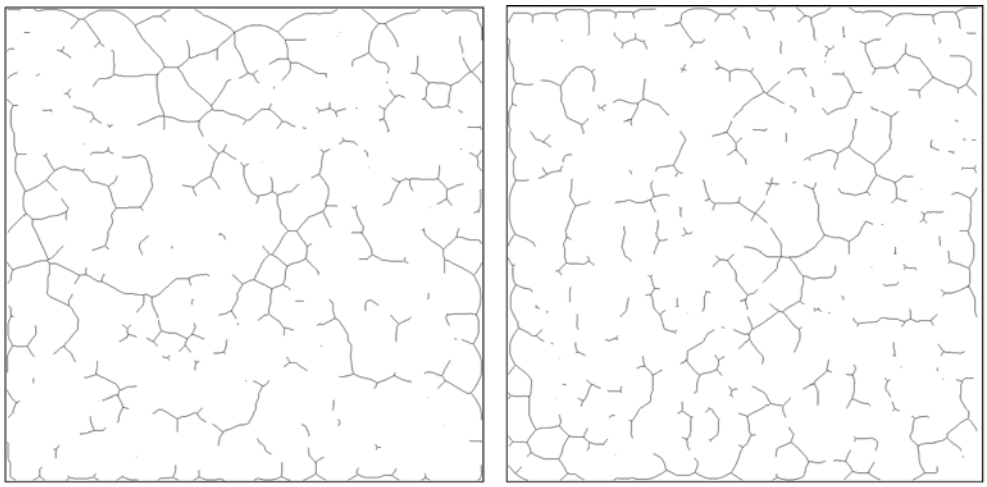

Fig. 11. Skeleton of pore space in 'dynamic' and 'random' packed and hydrated cements (Fig. 7).

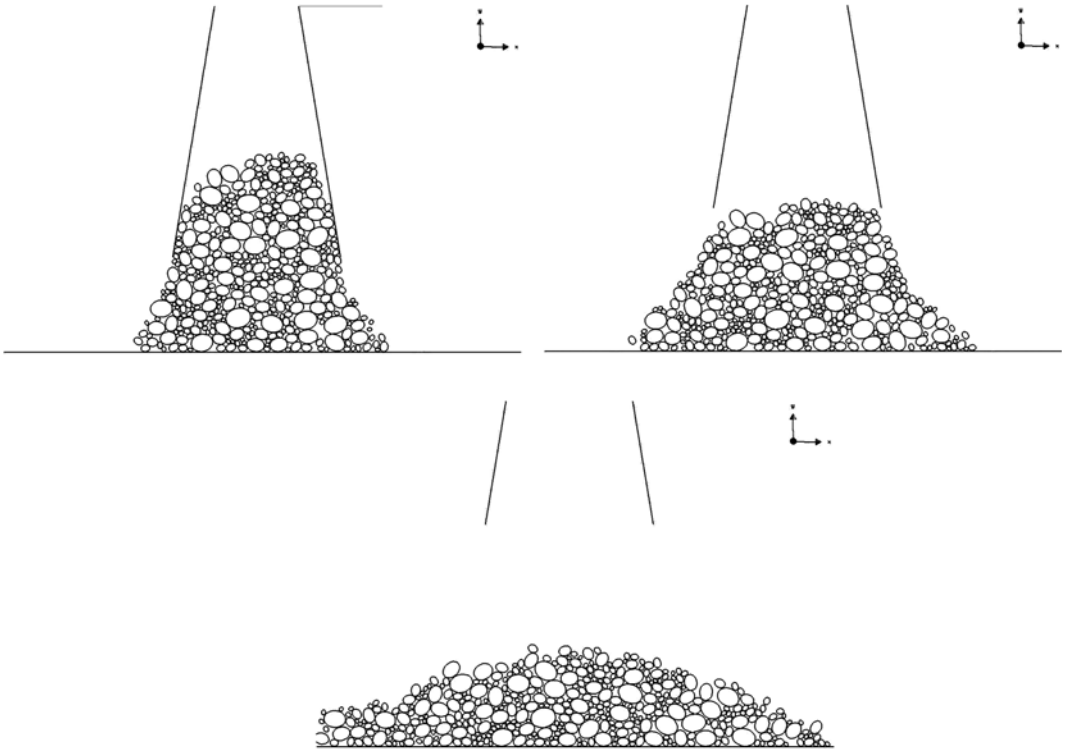

Fig. 12. Stages in the slump test as simulated by HADES

6. Practical DEM approaches in concrete technology

Three operational systems have been developed at Delft University of Technology for application to cementitious materials, SPACE, HADES and HYMOSTRUC3D. The last is an RSA system; the

other two are concurrent ones. Fundamental in all applications of DEM is that the configuration sensitivity involved in the tapped information should match that of the "schematization of reality" provided by the computer simulation system; otherwise operational potentials of the system will be violated, as explained and illustrated in this paper. Hence, instead of promoting a particular system, we do so with respect to *proper exploitation of any system*, so that the alchemy trap is avoided. Note that this paper is therefore not targeting to survey the available DEM systems in concrete technology; readers particularly interested in this sort of information are referred to van Breugel (2004) for some of the RSA systems in vogue nowadays. As to various types of concurrent algorithms for particle dispersion in concrete technology, a limited number of references are given in this paper. It goes without saying that any surveying of relevant developments outside the concrete technology field is contradicting the targets of this article. Nevertheless, for a single reference, see Williams and Philipse (2003), offering an extensive number of references to such developments outside the concrete technology field. Tüzün and Cleary (2006) and O'Connor (1996) also offer such information. Additionally, "Google" offers an enormous amount of information on a wide variety of DEM approaches.

Some typical and practical (thus, 3D) examples in concrete technology where RSA and concurrent systems will score differently will be presented in what follows.

6.1. Optimum aggregate packing

Most obvious example is simulating the dense random state of *aggregate packing* in concrete. This is impossible by RSA systems, so any comparison between the systems is impossible. However, the different concurrent algorithms also do not lead to the same maximum density as found in concrete mixtures. As mentioned earlier, SPACE application yielded proper correspondence to jammed state densities between 72-74% of various continuously graded aggregate mixtures of fluvial origin (Stroeven and Stroeven 1999, 2001). Volume densities of cementitious binders at (very) low water to cement rations are also outside the scope of RSA systems. For another system quite similar to SPACE/HADES, see Fu and Dekelbab (2003).

6.2. Structure of the ITZ

Similar applications of DEM can be mentioned on micro level, where the ITZ plays an important role (Bentz *et al.* 1993, Stroeven and Stroeven 2001c, Grutzeck *et al.* 1993). ITZs are the result of a phenomenon called size segregation. It manifests itself in the fresh as well as in the matured state, as revealed in SPACE-generated model cements (Stroeven and Stroeven 1996b, Hu 2004). This cannot properly be accomplished by RSA systems. Also, analytical solutions based on Poisson fields of particles lead to improper solutions (Zheng 2000). Different gradient structures were explored in the ITZ for composition (density, porosity) and for configuration-sensitive features of material structure (mean free spacing, surface-to-surface spacing, and bond strength). Some supporting experimental evidence is available (Diamond and Huang 2001). Full exploitation of this size segregation mechanism, leading to elimination of the ITZ as the "weakest link" in high performance materials, will require proper conditions for *internal migration* of particles (workability, compaction energy), as was confirmed by computer simulation (Stroeven *et al.* 2006b). In this high performance range, it has been demonstrated that the ITZ extent for bond strength significantly increases in the lowest water to cement ratio range (Stroeven 1999). Moreover, bond

strength can significantly exceed bulk value. This is well known from experiment testing on such HPCs, whereby elimination of the ITZ as weakest link can dramatically enhance brittleness of concrete. On engineering level, a multi-connected, relatively (dense) stiff and strong skeleton is formed. This should have obvious and dramatic effects on composite strength; topics that should be covered in the near future by concurrent algorithm-based systems.

6.3. Mechanical performance

A next major field of application of DEM encompasses efforts to simulate *mechanical performance* of concrete. One of the well-known solutions is the so-called numerical concrete (Zaitsev and Wittmann 1977) (based on the RSA system developed by Roelfstra (1989)). Other examples can be found in (Mościński *et al.* 1989, Markausas and Kačianauskas 2006, Tsunekawa and Iwashita 2001, Hentz *et al.* 2004a, 2004b). Two-dimensional sections of SPACE-generated 3D *meso*-structural concretes (aggregate grains with different grain size distributions in a matrix) subjected to tensile stresses have been analyzed by finite element approach (Stroeven *et al.* 2002). Damage evolution started as a highly structure-sensitive process, so, RSA systems would produce biased information. But this dependency on details of material structure (configuration) declined with global strain to which the concrete was subjected. Structure-sensitivity will be increased when also *shrinkage* is included. This is due to surface-to-surface spacing being a major parameter (with negatively skewed density distribution!) in this process. Shrinkage gives rise to premature cracking or to high residual stresses.

The post-ultimate branch of the load-displacement curve in these tests was found influenced by composition more than by configuration. Opening up of the macro-crack will be predominantly governed by the tortuosity of the crack, and the residual, diminishing, strength capacity, of course. Tortuosity has been analytically demonstrated a characteristic primarily relying on volume fraction of the aggregate (Stroeven 2000). Hence, fracture energy will also be a property with very low structure-sensitivity, as indeed reflected by experiments (Stroeven and Babut 1986). A practical consequence is that the associated RVE will have roughly the same dimensions as for, say, Young's modulus (RILEM 2004). Summarizing, numerical concrete based on RSA systems should concentrate only on more advanced states of damage evolution.

6.4. Workability, compactability

Another field of application is workability testing. A wide rage of test methods for workability has been developed, some for only specific situations (Koeler and Fowler 2003). Correlation between outcomes of such tests can only be roughly indicated for a limited number of methods. Application of DEM offers a way of enhancing insight into material behavior under various testing conditions, so that correlations might be established in the near future. Specific concurrent algorithms have been developed for simulation of flowing particles (O'Connor *et al.* 1997, Ansell and Dickinson 1986, Li *et al.* 2006, Klosek 1997, Puri and Uomoto 2002). Nevertheless, HADES can do this for arbitrarily shaped aggregate particles, too. As an example, Fig. 12 depicts a series of stages of the popular slump test in a 2D set up. Since particle configuration seems an important parameter, it can be emphasized that RSA approaches would lead to biased results.

6.5. Durability performance

A next field of major importance is *durability simulatio*n. In the first place, DEM is employed to simulate complex pore space, whereupon its spatial features are assessed that could be used in simulating transport phenomena. The de-percolation phenomenon, accompanying concrete maturation and governing transport properties of the material, is intimately associated with the morphological and topological characteristics of pore structure. The influences of water cement ratio and cement fineness level on the de-percolation threshold porosity can and have been investigated in this way. The structural evolution of pore space has been extensively studied in hydrating SPACE-generated model cement pastes and concretes on the basis of stereological spacing parameters (Hu and Stroeven 2005). Alternatively, similar approaches can be mentioned by other systems, including RSA ones.

A recent study (Chen *et al.* 2006, Chen 2009) with SPACE-generated fresh cement paste mixtures, subjected to hydration with HYMOSTRUC3D algorithm, provides information on technological influences on the extension of the ITZ for specific structure characteristics or material properties (such as global bond capacity) and on Torquato's probability density functions of the nearest surface-to-surface spacing and of the mean free spacing among aggregate particles. This would basically allow developing physical models for the *interconnected ITZ network* as a function of these technological parameters. In the range of conventional concrete qualities, this would be the more porous and weaker part of the material body, so that pore connectivity studies for durability purposes employing mathematical morphology operators could focus on this network structure. So far, this study demonstrated the connected pore fraction to be restricted indeed to a narrow zone close to the aggregate grain's surface (Fig. 13). This is highly relevant for durability studies. Alternatively, this three-phase structure composed of the interconnected ITZ network, matrix

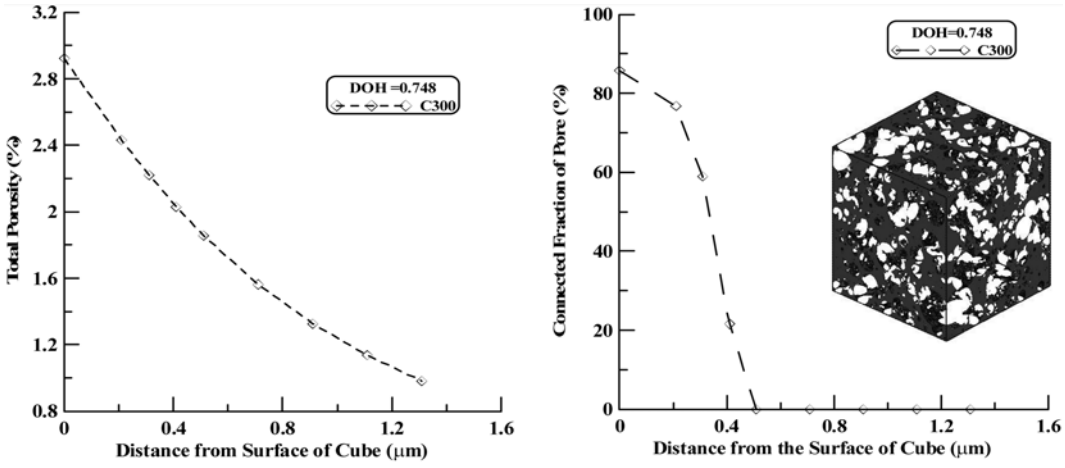

Fig. 13. Connected porosity (bottom) is restricted to a narrower zone (0.5 μm) in the ITZ of SPACE-generated paste (w/c=0.3; Blaine fineness 300 m^2/kg) between aggregate grain surfaces (container walls) than total porosity (top: zone of 2 μm) at about 75% degree of hydration (DOH). Maximum grain size in the simulation is reduced to about 50% with respect to that of the actual cement. Aggregate grain surface is at the left. Cube specimen (insert: pores in black) with rigid boundaries is investigated by serial sectioning and 3D reconstruction (Chen *et al.* 2006; Chen 2009).

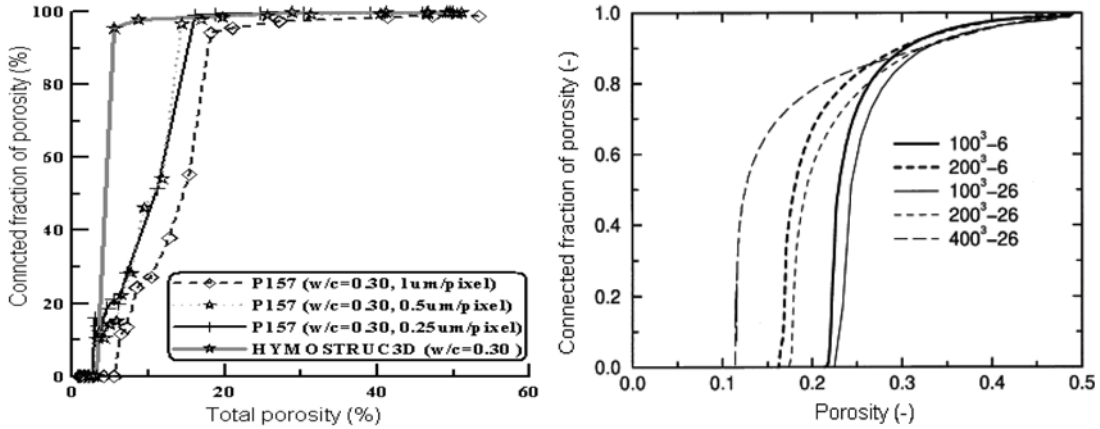

Fig. 14. Evolution of pore de-percolation during hydration (versus porosity), at the left for model cement pastes of which the fresh states were generated by HYMOSTRUC3D and by SPACE [2], and at the right according to Garboczi and Bentz (2001). Influence of resolution is also depicted (100^3, 200^3 and 400^3 correspond to a resolution of 1, 0.5 and 0.25 μm/pixel, respectively).

pockets of bulk cement paste, and dispersed aggregate particles could be subjected to advanced finite element approaches for material optimization purposes. Fig. 14 indeed illustrates that outcomes of the various systems as to this de-percolation process, so crucial for durability simulation estimation, are different. As earlier stipulated for damage evolution, the dependence of the de-percolation *process* on particle configuration diminishes during maturation. This indicates that the so-called percolation threshold is only weakly configuration sensitive, so that biases in outcomes of RSA systems will be reduced accordingly.

7. Conclusions

The two *physical discrete element modeling approaches* to cementitious composites, *i.e.*, sequential random addition and concurrent algorithm-based concepts *potentially* have their own merits and reasons for exploitation. In an economic sense, concurrent and RSA systems in concrete technology are probably quite comparable, provided *use is carefully restricted to the respective domains of usefulness*. The domains deal with different schematizations of reality. The operational potentials of RSA systems are limited to material performance of low structure-sensitive nature, laying only weak demands on the schematization of reality. The operational potentials of concurrent algorithm-based systems in the concrete technology field basically cover the full range of configuration or structural sensitivities, because of the realistic representation of reality with respect to particle spacing.

Despite the materials scientist's inability to characterize and describe cementitious materials comprehensively, this cannot be a proper reason to classify physical discrete element modeling of such materials as low technology. Concurrent algorithm-based DEM systems allow schematization of reality to be quite advanced, exploiting the operational potentials in an optimum way in a search for quantitative relationships between technological parameters and structure-sensitive performance, explicitly encompassing durability issues. This also gives answer to the question on alchemy raised

in this article. Provided the researcher complies with the materials science principles outlined, modeling by either RSA or concurrent algorithm-based systems should be awarded as sound scientific approaches, not leaving a fishy flavor of alchemy. Contrary, violating these principles by searching to exploit the limited potentials of an RSA-based system outside its domain of the structure-insensitive or low structure-sensitive properties should be classified as alchemy-like, and not just in metaphoric sense, since it would not be based on the present state of scientific methodology.

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