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RSA vs DEM in view of particle packing-related properties of cementitious materials

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Abstract. Various systems for simulating particulate matter are developed and used in concrete technology for producing virtual cementitious materials on the different levels of the microstructure. Basically, the systems can be classified as two distinct families, namely random sequential addition systems (RSAs) and discrete element methods (DEMs). The first type is hardly being used for this purpose outside concrete technology, but became popular among concrete technologists. Hence, it is of utmost relevance to compare the two families in their capabilities, so that the reliability of produced data can be estimated. This paper pursues to do this on the basis of earlier published material of work performed by a succession of PhD students in the group of the second author. Limited references will be given to external sources.

Keywords: cementitious materials; aggregate; hydration; porosimetry; permeability; structure-sensitivity

1. Introduction

Concrete is a particulate material on the different structural levels. Hence, packing of the relevant particles is a phenomenon that underlies the material's properties. Packing can be and has been studied experimentally. However, this is a time-consuming and laborious operation. So, doing this in virtual reality is at least attractive in economic sense. Provided the packing characteristics can be simulated realistically, it would also be a reliable alternative.

Random sequential addition (RSA) algorithms are popular for this purpose in concrete technology, far more than outside. Yet, the discrete element model (DEM) is already for four decades or so on the market (Cundall and Strack 1979) and is widely acknowledged to offer a far better quality virtual concrete. A survey of RSA and DEM systems in vogue in concrete technology can be found in (Stroeven *et al.* 2009a, 2010). This primarily concerns hardened concrete. For the modelling of flow of fresh concrete by DEM, see e.g., Mechtcherine and Shyshko (2007). Still, a mutual comparison of such systems is not targeted in this paper. Instead, the characteristic and more fundamental differences between DEM and RSA will be highlighted and the impact of this on properties will be discussed. Due to aforementioned superior quality of DEM simulation, it is also relevant showing the degree of misfit in RSA estimates. Examples and illustrations are mostly selected from published papers based on research performed earlier in the group of the second author by successive PhD students. This will involve simulations and physical experiments on different structural levels. Outside the concrete technology field this is quite trivial matter, yet researchers in this very field pursue using RSA systems seemingly unaware of the impact that will have on various material properties.

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2. Conceptual approach

RSA is a particle deposition strategy. Random numbers are employed for the deposition of a particle inside container space, starting from the largest one to speed up the process. However, when packing density increases, particle overlap will become a major phenomenon. Specifically, when a particle is deposited on a position leading to overlap with a particle earlier placed in the container space, this operation will be rejected and the particle is removed from the container. Then, new coordinates are required for repositioning the particle. This procedure has two serious consequences:

1. The number of rejections will dramatically rise upon increasing the density. This leads to a maximum achievable particle density far below the practical range for aggregate packing (Williams and Philipse 2003, Ballani 2005, He 2010). In such practical situations, one is confronted with the dense random packing state. And even for simulating cement particle packing at (very) low water to cement ratios relevant for (super) high performance concrete, the loose random packing state should be achievable, which is almost impossible by RSA. This is a practical argument against using RSA for packing simulation of aggregate and even for cement particles at (very) low water to cement ratios.

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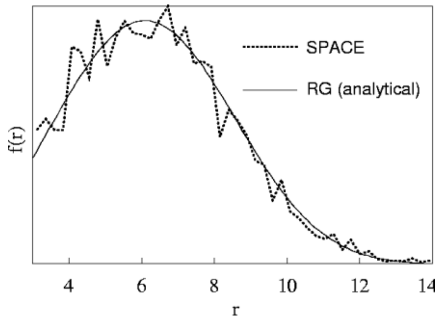
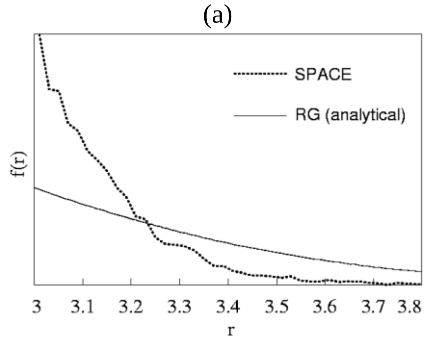
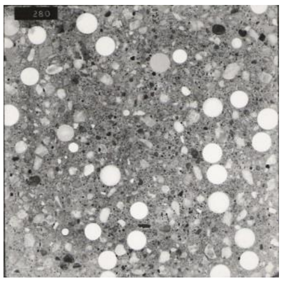


(a)

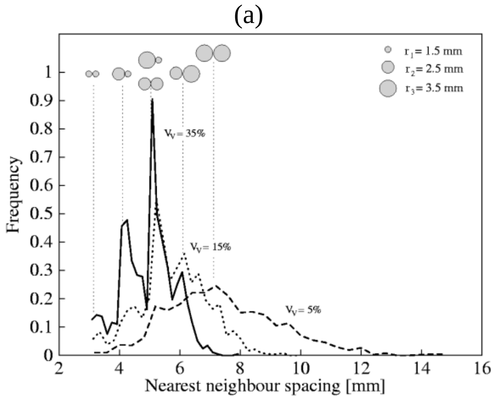


(b)

Fig. 1 Deviations between predictions on nearest neighbor density distribution, $f(r)$, at 1% (a) 30% (b) by volume of aggregate obtained by a random generator (RG) (RSA algorithm), respectively, and by a concurrent algorithm based DEM (SPACE) computer simulation system (Stroeven 1999, Stroeven and Stroeven 1999a)



(a)



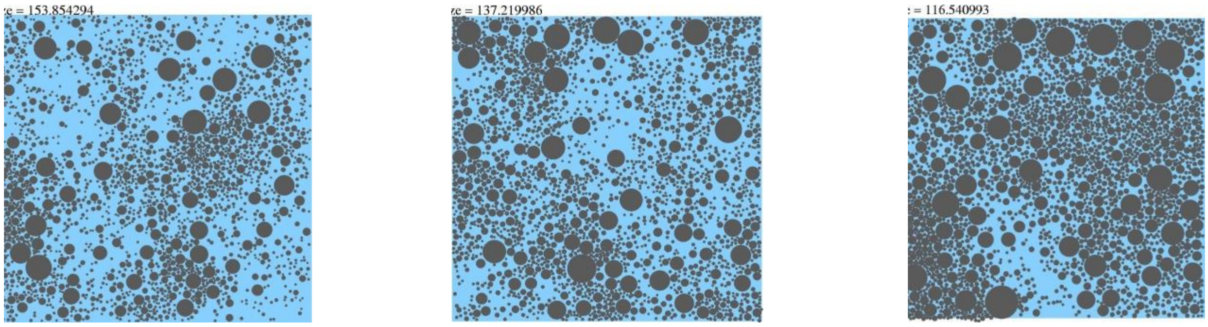
(b)

Fig. 2 (a) Section (200x200mm) of 250 mm concrete cube reveals clustering tendency among grains in large aggregate fraction of 16 mm mono-size ceramic spheres (9.2% by volume) (Stroeven 1973). (b) 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)

2. A rejection is necessary when the two particle centers come too close. This would lead in the real material–realcrete–to a (near) contact situation between particles, so, to patch formation. However, the regeneration leads-when seen for a large number of rejection and regeneration cases-to positions that are by chance more evenly distributed in the space between neighbour particles. Hence, such a 3D dispersion of particles is at growing density to an increasing degree biased with respect to particle dispersion. Williams and Philipse (2003) state therefore that "any relation between these RSA packings and an experimental granular packing is at best tenuous". This is a fundamental argument against using RSA for the simulation of properties that depend on particle dispersion. Such properties are denoted structure-sensitive, which holds for the majority of properties concrete engineers are interested in. The production of real concrete implies particle interferences on the different levels of the microstructure. Hence, this phenomenon should also be involved in producing the virtual representations of these materials. As we have seen above, this phenomenon is ignored in RSA simulations. Instead, it is fundamental in the discrete element model (DEM), whether of static or dynamic nature.

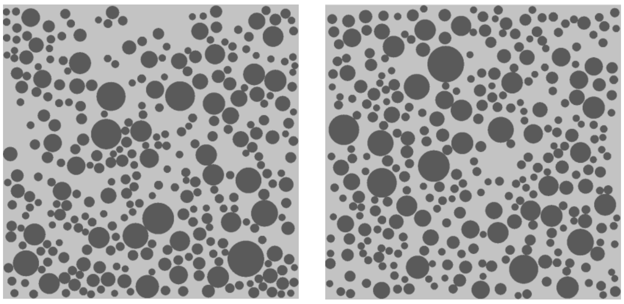
DEM is a particle interference strategy. Particles are not one-by-one deposited inside a container. Instead, all particles are jointly dispersed in an enlarged container. Hence, RSA algorithms could be used in this stage. DEM starts when all particles have found positions in this enlarged container. In a dynamic system, the particles are set to linearly move (and with non-spherical particles to rotate), as a result colliding among each other and with the container sides. The container is gradually reduced in size until the designed particle density is obtained. The dynamic stage is thereupon stopped; particles have reached their final destination. In a static system, particle positions are only locally shifted to eliminate overlap during the process in which the system is gradually squashed. For a detailed description, see e.g., O'Connor (1996), Stroeven (1999), Williams and Philipse (2003) and Mechtcherine *et al.* (2014). These DEM systems produce virtual materials–compucrete-that in accordance with the real material, reveal particle clustering or patch formation on meso- as well as on micro-level (Diamond and Thaulow 2006, He *et al.* 2009, Stroeven *et al.* 2009a). This phenomenon is depicted by Figs. 1-3. The starting of patch formation is reflected by the highly sensitive nearest neighbor spacing.

Fig. 1 demonstrates the gap in nearest neighbour spacing distribution of RSA and DEM estimates to significantly grow between 1 and 30 % by volume of particles. Fig. 2 specifically demonstrates that in a particle mixture of three mono-size grain fraction, peaks in the nearest neighbour distribution arise at increasing density due to particle interferences in the DEM simulated virtual material. A randomly selected section of real concrete containing spherical ceramic aggregate as largest fraction also reveals an "uneven" (so, partly patched) distribution of the grains. Fig. 3 demonstrates the formation of patches in the fresh cement grain structure at increasing density. Particle attraction is not implemented in this case.



(a) *w/c*=0.50 (b) *w/c*=0.42 (c) *w/c*=0.34

Fig. 3 Sections of cubes with rigid boundaries of DEM-produced fresh cement paste models at increasing particle density. Material density is obviously fluctuating, despite particle attraction (or repulsion) not being included in the dynamic packing process by SPACE. As a result, “patches” can be distinguished (Diamond and Thaulow, 2006; Stroeven *et al*. 2009b)



(a) (b)

Fig. 4 Range of sizes of cylindrical particles packed in a container with rigid boundaries at 0.4 areal fraction. (a) a section of a DEM (SPACE)-produced tile (by dynamic mixing), (b) a section from a tile with the same ensemble of particles obtained by RSA procedure. Patch formation is properly simulated by the SPACE system

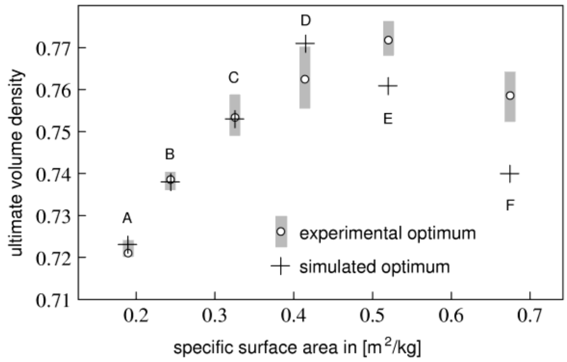


Fig. 5 Comparison of the density at the jammed states of different mixtures of river gravel aggregate compacted in standard 8-liter cylinders, and of SPACE-generated spherical aggregates with similar grading characteristics. Mixtures A to F have an increasing specific surface area (so, are finer-grained), with mixture E close to the Fuller one. Correspondence is satisfactory. For experimental details, see (Donker 1998, Stroeven 1999, Stroeven and Stroeven 1999b)

3. Experiments and simulation on meso-level (aggregate grains)

3.1 2D simulation by RSA and DEM

Let’s start simple with a 2D example as presented in Figs. 4(a)-(b). This can already qualitatively and visually demonstrate differences between virtual materials simulated by RSA and by DEM indicated in Section 2 of this paper (Stroeven *et al*. 2009a). Of course, the example can be equally conceived as packed “particles” on meso-level (aggregate) as well as on micro-level (fresh cement). We will elaborate the quantitative differences between DEM and RSA packing when Fig. 4 is later interpreted on micro-level.

3.2 Maximum packing density in experiments and in DEM simulations

Fig. 5 presents a comparison between realcrete and compucrete, the latter simulated by DEM (SPACE). Real mixtures of river aggregate were on a standardized way compacted in 8-litres cylindrical molds. Mixtures of spherical particles conforming to the same sieve curves were compacted by the SPACE system in cubic containers with rigid boundaries. Mixtures *A-F* have an increasing fineness, whereby *E* is close to a Fuller distribution. This type of virtual experiments cannot be executed by RSA because of the required dense random packing states. Obviously, simulation by DEM leads to satisfactory agreement.

DEM-based virtual concretes with river and crushed rock aggregates have been used for estimating elastic properties (He *et al.* 2012). At moderate densities, this could also have been achieved by RSA approach due to the low structure-sensitivity involved. However, estimation of fracture properties, as also conducted on DEM-based material models (He *et al.* 2011), would have led to biased outcomes when based on RSA approaches.

A second example of DEM application to aggregate simulation has been realized by HADES, the successor of SPACE, which can pack arbitrarily shaped particles from the dilute to the dense random state (He *et al.* 2009, He 2010, Stroeven *et al.* 2011). Fig. 6 shows examples of packing differences among crushed rock and river gravel aggregate composed of a variable mixture of fine and coarse aggregate fractions. Hence, shape as well as composition effects in aggregate mixtures were visualized

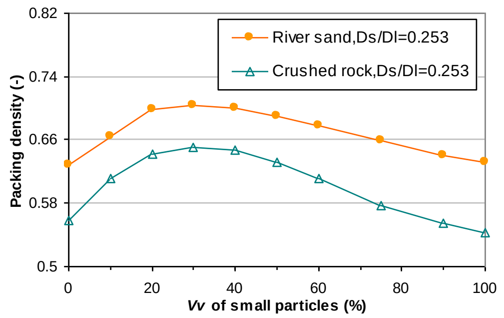


Fig. 6 Maximum packing density versus composition of bimodal mixtures for different aggregate types (shapes) obtained by virtual packing experiments (Ds and Dl: sieve sizes of small and large particles, respectively)

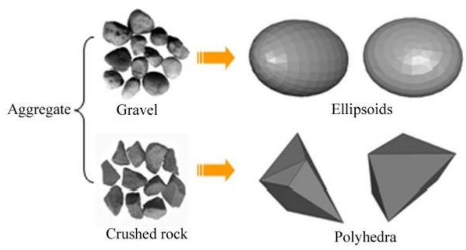


Fig. 7 Two families of aggregate shape to simulate river aggregate and crushed rock aggregate, respectively

in this study. The high densities cannot be realized by RSA, while shape effects cannot be studied even by most DEM systems because based on spherical grains. The grains of the crushed rock aggregate were polyhedron-shaped, whereas those of the river aggregate had an ellipsoidal shape, as revealed by Fig. 7. Fig. 8 visually illustrates some loose random packed states of several typical shapes.

3.3 Particle dispersion by DEM and in experiments

Another comparison is depicted in Figs. 9(a)-(c) (Stroeven 1999, Stroeven *et al.* 2008). 200 mm boundary-free concrete cubes in which the largest sieve fraction was replaced by mono-size ceramic spheres of 16 mm diameter were subjected to serial sectioning and 3D reconstruction. All ceramic spheres were cut three times (thickness of tile and saw cut amounted, respectively, about 11 and 3 mm). All section images were photographed, whereupon the coordinates of three points on each perimeter of particle sections were measured on full-size transparencies (Stroeven 1999). 3D reconstruction allowed the analysis of the spatial dispersion of the ceramic spheres in the concrete. The displayed example contained 22.6% ceramic coarse aggregate by volume. The cube in Fig. 9(b) shows the simulated virtual material, consisting of a transparent matrix (containing the rest of the aggregate grains) and the spherical ceramic grains. The section in Fig. 9(c) is from the realcrete cube. Fig. 9(a) shows the distribution of the nearest neighbour distance, Δ_3, of the ceramic spheres obtained in the physical experiments and in the simulation approach. In the realcrete, these 16 mm ceramic spheres replace the largest sieve fraction of normal concrete. The realcrete's curve is obtained by serial sectioning and 3D reconstruction. Similarity is quite reasonable: note that the realcrete's curve should start from 16 mm upward! Hence, the differences are primarily due to the unavoidable inaccuracies imposed by the sawing operation. The relatively large number of small Δ_3 values point again in the

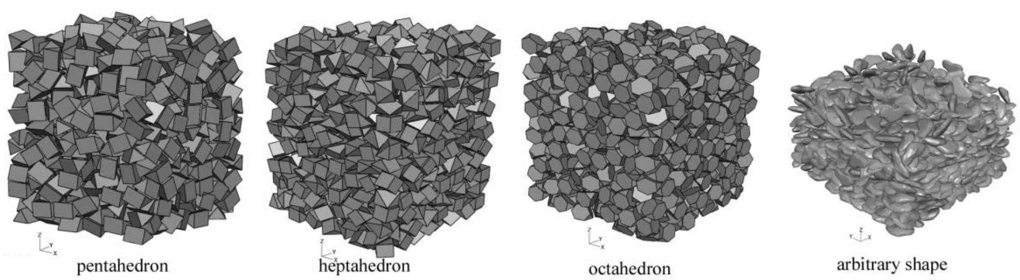
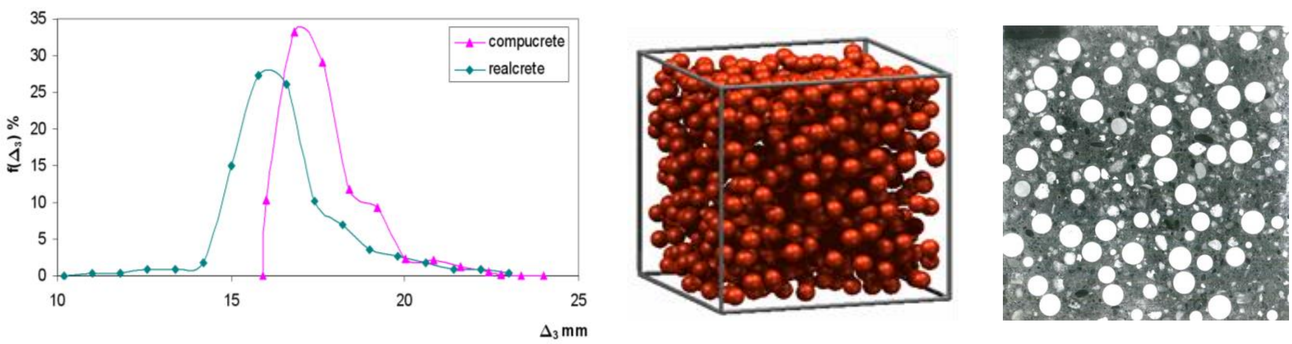
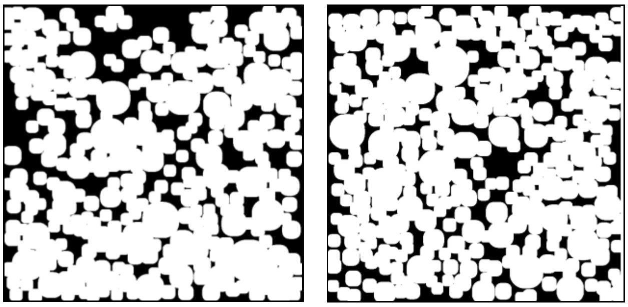


Fig. 8 Simulated mono-size loose random packing states of particles with various shapes



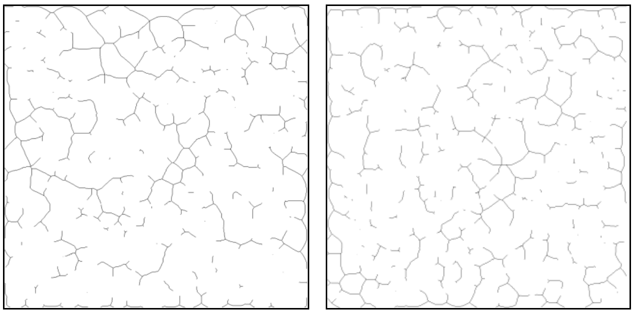
(a) (b) (c)

Fig. 9 (a) Frequency distributions of the nearest neighbor, Δ_3, among 16 mm ceramic spheres in a 200 mm sample, (b) virtual material, (c) real material



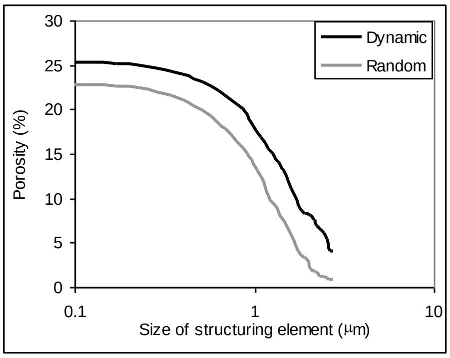
(a) dynamic DEM (SPACE) (b) RSA

Fig. 10 Simulated (dynamic DEM: left; RSA: right) hydrate structure in cement paste, additionally revealing pore space in the equally long matured 2D cements of Fig. 4

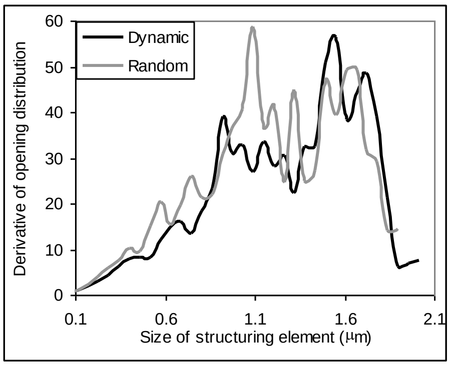


(a) dynamic DEM (SPACE) (b) RSA

Fig. 11 Skeleton of pore space in 'dynamic' (DEM) and 'random' packed (RSA) and hydrated cements of Fig. 4. The latter network is more uniform



(a) Cumulative porosity distribution



(b) Pore size distribution

Fig. 12 The hydrated cement pastes (material structure visualized in Fig. 4), of which the fresh states are generated by SPACE ('dynamic' DEM) and by RSA procedures (denoted as 'random'). Use has been made of the opening distribution technique (Hu 2004, Hu and Stroeven 2006)

direction of patch formation. This cannot be simulated by RSA.

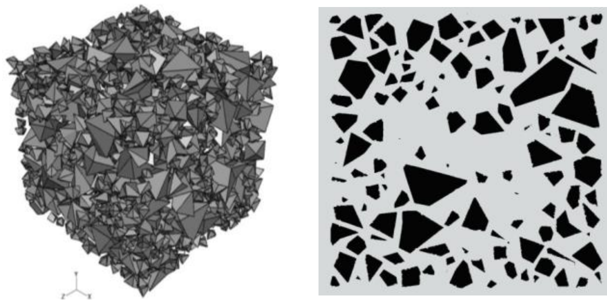
As stated earlier, patches develop in the dispersion of packed aggregate. This can be properly simulated by DEM (Stroeven *et al.* 2009b, Stroeven and He 2009), however not by RSA. We will come back to this topic in what follows.

4. Experiments and simulations on micro-level (cement grains)

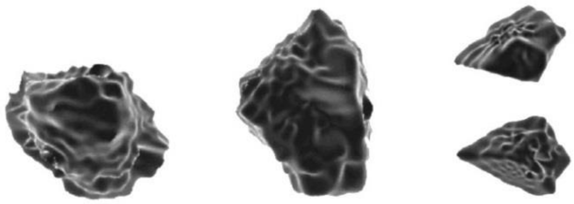
4.1 2D simulation by RSA and DEM

The simple example of 2D simulation of particle packing illustrated by Fig. 4 is interpreted in the present case as 2D dispersed cement grains in the fresh state in a 100 μm container. Visual differences between the respective specimens can be quantified by e.g., the nearest neighbor distribution, $f(\Delta_3)$ (Fig. 9). Mean values of both distributions are 0.236 μm (left) and 0.262 μm (right). About 10% difference is due to more realistic patch formation or particle clustering.

For hydration simulation in this 2D illustrative example, a simple dilation algorithm is used for the two simulated fresh cement distributions, leading to proportional expansion as a result of the hydration products (Fig. 10). No particle interferences are considered herein. The resulting pore systems after similar hydration duration can now be analysed. A first impression of the typical differences that are due to the biased particle dispersion in the RSA system is given by Fig. 11, presenting the skeleton of pore space. Further, typical results are plotted in Fig. 12.

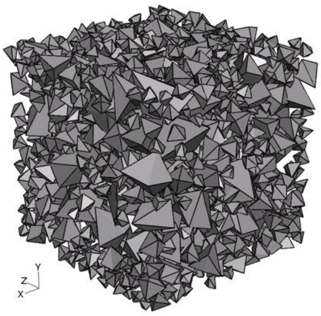


(a) (b)

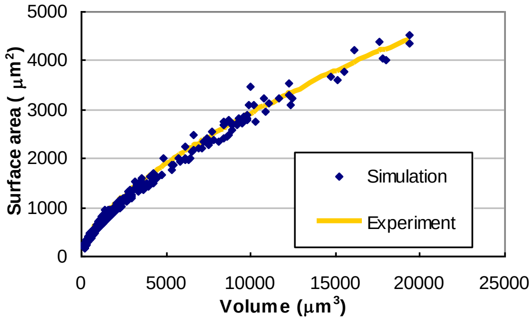


(c)

Fig. 13 (a) Visual model of HADES-compacted octahedron-shaped cement grains, (b) image of section through package, revealing patchy structure (He 2010), (c) the shape of real cement grains (Garboczi and Bullard 2004)



(a) Structure of compacted cement grains



(b) Experimental regression results

Fig. 14 Surface versus volume of 1000 multi-size polyhedral particles in 10-50 μm range packed by DEM package, HADES

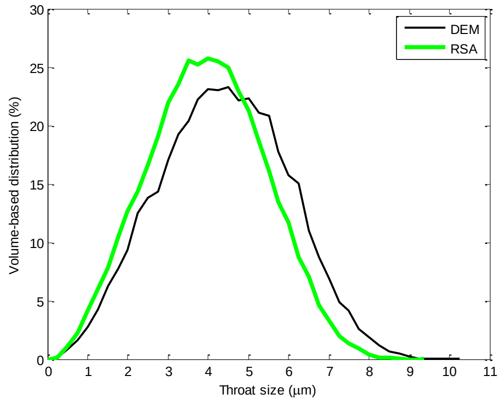
Even this simple example reveals the effects of the inherent bias of the particle distribution in RSA approaches. Impact on a so called structure-insensitive property like porosity is small, however, not to be neglected. On the critical pore size, a structure-sensitive property, which can be derived from Fig. 12(b), the effect is significant (as can be imagined from the completely different graphs); for detailed information, see Hu (2004).

4.2 Packing of cement grains – DEM vs experiments

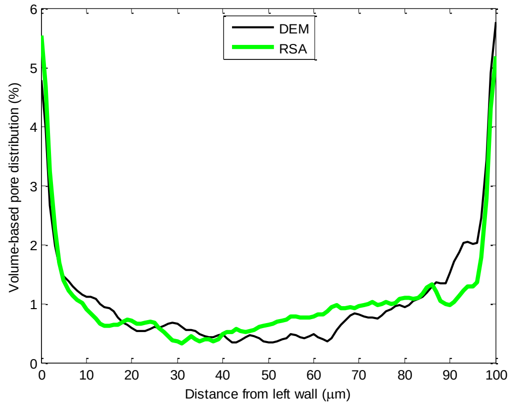
As could be expected, the cement grain structure as depicted in Fig. 13 also reveals significant patch formation, which could only be marginally represented by RSA approaches. Moreover, the DEM system HADES can simulate the fresh cement structure with non-spherical particles, which is also impossible by many DEM systems. The used shape of the cement grains is in agreement with experimental findings (Garboczi and Bullard 2004). The ratio of surface area to volume of the cement grains (polyhedra) is made in agreement with experimental findings (Garboczi and Bullard 2004), as shown in Fig. 14.

4.3 Pore de-percolation during hydration by RSA and DEM

The pore size distribution differences found in the 2D analysis are supported by a 3D analysis. Fig. 15 depicts typical differences observed between RSA- and DEM-produced pastes. It should be noted that the simulated size range of the model cement is about three times smaller than in reality. Hence, observed differences should be roughly multiplied by a factor of three.



(a) Larger size range by DEM



(b) Wider ITZ by DEM

Fig. 15 Differences in pore size distribution between DEM and RSA simulation (Stroeven, 2013)

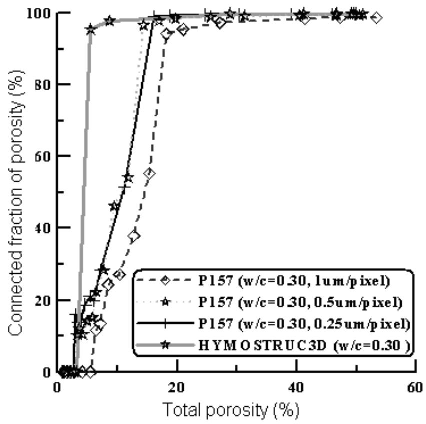


Fig. 16 Evolution of de-percolation of pore structure during the hydration process (plotted vs porosity) for the model cement paste generated by SPACE (DEM) and by HYMOSTRUC3D (RSA) (Chen *et al.* 2006)

Since cement particles are distributed more evenly than follows from the more realistic DEM approach, the resulting pore size distribution is also negatively affected: RSA presents a too narrow size range. This will have impact on the de-percolation process too, as proven by Fig. 16. Fig. 16 is based on identical cement pastes (with respect to particle size distribution and water/cement ratio). The fresh virtual pastes were produced by Hymostruc3D (RSA)

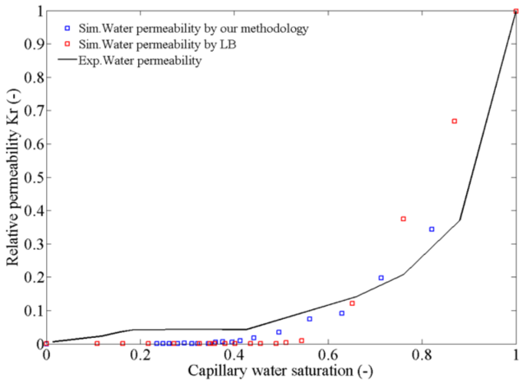


Fig. 17 Effect of stagnant water content in pore system in virtual DEM-based hydrated cement paste on relative permeability K_r. Experimental data for hardened concrete with various amounts of stagnant water in the pore system is from (Kameche *et al.* 2014). LB represents Lattice Boltzmann method used for permeability calculation in RSA-based structure in (Zalzale *et al.* 2013). DEM data are closer to experimental ones than those obtained by RSA system

and SPACE (DEM), respectively. Thereupon, the fresh pastes were simulated by vector approach with Hymostruc3D to be able using Ye's (2003) serial sectioning and 3D reconstruction method for assessment of pore characteristics.

Hence, the only differences in Fig. 16 are due to the dispersion of the fresh cement mixture. Obviously, the more even dispersion produced by the Hymostruc3D (RSA) system led to a narrower range of pore sizes, as we have seen, which caused a delayed and more sudden de-percolation process. In the DEM approach by SPACE system we have a wider range of pores that caused a more gradual de-percolation in the pore network system. Hence, the structure-sensitive process is significantly biased as produced by the RSA system. The de-percolation limit is far less structure-sensitive, so that at higher sensitivity the estimates from both systems were not too much different.

4.4 Permeability of concrete containing various amounts of stagnant water – DEM vs experiments

Unfortunately, concrete permeability is a function of geometrical and topological characteristics of the pore network system that are structure-sensitive to different degrees. Hence, permeability estimates will be biased to an unknown degree when based on RSA systems. Virtual cement produced by DEM (HADES) and hardened by XIPKM (hydration simulation by the improved vector approach) (Le *et al.* 2013) was analyzed by DRaMuTS (robotics system for pore delineation) (Stroeven *et al.* 2012) and by SVM (life science method for measuring the 3D pore size distribution and the 2D pore throat distribution) (Stroeven *et al.* 2010), yielding a pore network structure of quantified topological and geometry properties. Next, this pore network structure was assumed partly filled by water, representing practical conditions. The permeability estimates were found close to recently published experimental data for concrete containing various amounts of water (Kameche *et al.* 2014), as shown in Fig. 17. In addition to having validated the aforementioned "building blocks" of the methodology in separate publications, this constitutes an overall validation for the DEM-based approach (Li *et al.* 2016, Li *et al.* 2017). RSA-based simulation results (Zalzale *et al.* 2013) are more away from the experiments (Kameche *et al.* 2014) as additionally revealed by Fig. 17.

5. Discussion

The practical and fundamental deficiencies of the RSA approach mentioned in the introduction are well-known, however, are also ignored in data presentations of the frequently used RSA-based systems in concrete technology. This paper demonstrates the occurrence of such deficiencies by comparing a series of cases with outcomes of experiments and DEM approaches dealing with properties of various degrees of structure-sensitivity. It also offers insight into the character and magnitude of the impact of the deficiencies. Hence, in many practical cases, RSA cannot be used at all because of too low packing density capabilities. This is certainly the case when dealing with aggregate packing on meso-level or binder particle packing at (very) low *w/c* ratios relevant for (super) high performance concrete.

However, far more serious is the effect in cases where RSA yields estimates that are inevitably biased by the underlying fundamental deficiency in producing unrealistically dispersed particles. This is certainly the case when porosimetry is at stake for estimating permeability properties in the framework of durability research. In the latter case, experiments are commonly performed by MIP (or eventually WMIP). This leads to pore size estimates orders of magnitude too low (as demonstrated by quantitative image analysis); see Diamond (2000). This should be considered when comparing data on virtual and real cementitious materials (Stroeven *et al.* 2015).

Another shortcoming of experimental research into permeability is the uncertain level of water saturation in the pore system. So, the experimental data plotted in Fig. 17 should be approached with a certain degree of scepticism. The fully saturated state in particular cannot be reproduced even when storing concrete specimens for longer periods under submerged conditions. The same can be argued for the case of completely empty pores. Hence the experimental curve in Fig. 17 covers a narrower range than plotted. This would make the agreement between DEM simulations and experimental data even more striking. This should be part of the discussion when trying to validate data obtained on virtual cementitious materials as discussed herein.

6. Conclusions

In the discussion on DEM vs RSA in concrete technology, the following conclusions pertain:

- DEM has practical advantages over RSA, since the latter approach does not render possible simulating the associated packing states of dense random (aggregate) or loose random (binder) at (very) low water to cement ratios.

• For the estimation of structure-sensitive properties – so, properties depending on the dispersion of the packed grains - DEM is superior, due to the fundamentally biased dispersion reproduced by RSA procedures.

• Elastic properties are quite structure insensitive, so that also RSA systems can be used. However, the various fracture properties are structure-sensitive to different degrees requiring estimation by DEM systems.

• Geometrical and topological characteristics of the pore network structure in hardened cement paste are structure-sensitive to different degrees, so that the virtual reproduction by RSA is biased to an unknown degree, which therefore also holds for permeability estimates.

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