Journal of Zhejiang University-SCIENCE A (Applied Physics & Engineering)
ISSN 1673-565X (Print); ISSN 1862-1775 (Online)
www.zju.edu.cn/jzus; www.springerlink.com
E-mail: jzus@zju.edu.cn

Discrete element modelling approach to assessment of granular properties in concrete

Piet STROEVEN[1], Huan HE[†‡1,2], Martijn STROEVEN[1]
(*[1]Faculty of Civil Engineering and Geosciences, Delft University of Technology, Stevinweg 1, 2628 CN Delft, the Netherlands*)
(*[2]Faculty of Applied Sciences, University of Liege, Chemin des Chevreuils, 1, 4000 Liège, Belgium*)
[†]E-mail: H.He@live.com

Received May 11, 2010; Revision accepted Oct. 28, 2010; Crosschecked Dec. 10, 2010; Published online Jan. 18, 2011

Abstract: This paper presents the technological relevance of a concurrent algorithm-based discrete element modelling (DEM) system, HADES. This new system is the successor of SPACE that is limited to spherical grains only. It can realistically simulate the packing of arbitrary-shaped particles up to the fully compacted state. Generation of families of such particles, i.e., generally representing aggregate of fluvial origin and crushed rock, respectively, and the forming way of particulate structure are described. Similarly shaped particles are proposed for simulation of cement paste because of conformity with experimental results obtained by the X-ray tomography method. Technologically relevant territories inside and outside concrete technology are presently explored in this efficient, reliable, and economic way. Some results obtained by this DEM approach are presented.

Key words: Cementitious materials, Granular properties, Concurrent algorithm, Discrete element modelling (DEM), Shape, Particles
doi:10.1631/jzus.A1000223 **Document code:** A **CLC number:** TU528

1 Introduction

Cementitious materials are of particulate nature on different structural levels. The aggregate is compacted in the fresh concrete into the jammed state. It is a strong and hard material, under such conditions approximately taking up three-quarters by volume of the material body, providing normal concretes with high compressive strength. The stability of the skeleton is guaranteed by the cementitious “glue”, the cement paste. Moreover, the paste’s quality, which is directly influenced by its fineness and the water to cement ratio, governs the actual composite’s compressive strength level. Additionally, the paste gives the material tensile strength. Modern high performance concretes are produced at a low water to cement ratio, so the volume content of the cement in the paste may be as high as 60%. This is achieved by the addition of chemical and fine mineral admixtures. The latter can also be employed for replacing part of the Portland cement (PC) and can be of pozzolanic or inert nature. All composing parts of the material influence the engineering characteristics of the composite that will change as a function of time, in the first place as a result of hydration. However, this is also due to complicated interaction processes with the environment. Material optimization studies demand very large numbers of specimens. Traditionally, trial testing and structural research programs have been conducted to approach such problems, but it would be economically attractive to have reliable computer simulation methods available for this purpose.

The common discrete element computer simulation system in concrete technology is based on random generators to disperse inside the container aggregate particles on the meso-level in a cementitious matrix, or cement and eventually other types of mineral admixture particles on the micro-level in the watery environment during the fresh state. These

---

[‡] Corresponding author

systems are referred to as random sequential (particle) addition (RSA) systems. As stated elsewhere, they generate particles that are not spaced according to situations encountered in the actual material (Williams and Philipse, 2003; Stroeven and Guo, 2006). This is true for the particulate systems on both structural levels. As a result, the processes of pore de-percolation, underlying concrete durability, and damage evolution, governing the materials residual strength capacity, will be incorrectly generated. Biases will decline fortunately during such processes due to reducing structure sensitivity. Damage estimation was pursued by the RSA-based concept of "numerical concrete" (Wittmann *et al.*, 1985), which is RSA-generated concrete subjected to finite element (FE) analysis. Additionally, RSA systems cannot economically produce particulate systems with the aforementioned high volume densities. Therefore, we have applied the concurrent algorithm-based discrete element computer simulation system SPACE with success on both structural levels (Stroeven *et al.*, 2006; 2008; He *et al.*, 2008).

A drawback of such systems is that generally only spherical particles can be generated. For aggregate of fluvial origin this is not considered serious but for crushed rock aggregate or even for cement, this may lead to biased results. Aggregate grains with non-spherical form are known to lead to lower densities in the jammed state. This has implications for engineering strength. However, the impact on the "nodes" in the spatial pore network structure that governs hydraulic properties underlying durability performance could be more serious (Stroeven and Guo, 2006; Stroeven *et al.*, 2008; 2010). Realistic packing research on different structural levels by discrete element modelling (DEM) therefore also requires facilities to generate non-spherical particles. This is possible by HADES. With this package, particles can be of any shape and contacts are force-based rather than impulse-based, as in SPACE system (Stroeven *et al.*, 2006). 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. Some applications of HADES in concrete technology have been described (Guo *et al.*, 2007). This paper indicates some new typical fields which have been explored in this way. Similar types of investigations based on other concurrent algorithm-based systems can be found in (Jodrey and Tory, 1981; Ansell and Dickinson, 1986; Mościński *et al.*, 1989; Klosek, 1997; O′Connor *et al.*, 1997; Tsunekawa and Iwashita, 2001; Puri and Uomoto, 2002; Williams and Philipse, 2003; Li *et al.*, 2006; Markausas and Kačianauskas, 2006).

2 Discrete element modelling

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 (computer concrete)? Such questions must have been at the minds of those describing the first systems in the 1970s and 1980s, such as Roelfstra (1989), which is the basis of the "numerical concrete" concept of Zaitsev and Wittmann (1977). Basically, these models and some systems developed later in concrete technology rely on RSA algorithms (van Breugel, 1991; Bentz *et al.*, 1993; Meakawa *et al.*, 1999). In RSA systems, particles are placed proceeding from large to small on preconceived positions of a Poisson field (He, 2010; Zheng *et al.*, 2010). 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 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% with mono-sized spheres. In Williams and Philipse (2003) an upper limit of 38.5% for mono-sized spherical particles is mentioned, which is in qualitative agreement with Ballani (2005) where in most cases the production of compucrete with 40% mono-sized spherical aggregate failed. So, practical arguments ask for applications to low density grain mixtures only under such conditions. It is more feasible for RSA systems to produce a multi-sized particle packing. However, instead of having series of particles close together in compucrete, in conformity with Poisson point processes, on average a more uniform dispersion is obtained due to the static nature of the approach.

Clustering, a natural phenomenon in particulate matter (Stroeven, 1973; Diamond and Thaulow, 2006) is therefore very poorly represented by RSA systems. Conversely, the concurrent algorithm-based computer simulation systems SPACE and HADES imitate the production conditions of concretes and have been demonstrated realistically incorporating the clustering phenomenon in compucrete (Stroeven *et al.*, 2009a). In general, particle dispersion in RSA-based virtual concrete is biased, because it does not constitute a realistic representation of the real concrete (realcrete) (Stroeven *et al.*, 2009b).

The SPACE and HADES systems create compaction using a dynamic algorithm, which also imitates the production stage of the material, as mentioned above. 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 easily be included. Compaction of particles is realized in SPACE by a dynamic Newtonian motion algorithm. Particles move and collide to prevent overlap. Also in HADES, particles undergo linear and rotational movements. However, it is based on a contact mechanism that evaluates the interaction forces exerted between segmented surfaces of neighboring particles. For that purpose, guard zones are defined around each particle (Fig. 1). When the distance between two segments is less than the extent of this guard zone, interaction forces between two segments will be activated. The contact force is a function of the distances and areas of segments. Total force is calculated by integrating the function over relevant parts of the surfaces of the grains governed by the extent of the overlap area of the guard zones. For that purpose, the function is evaluated at a number of evaluation points similar to FE approaches. Meanwhile, several forces can be applied on particles, such as spring forces (representing a repulsive force between bodies), cohesion forces (representing attraction between particles), damping forces (incorporating energy losses in the system), and friction forces.

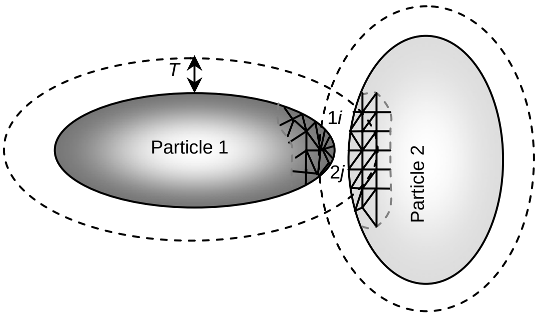


Fig. 1 Example of interaction between two particles
Surface tessellations in interaction zone are sketched. T is the guard zone thickness of a particle; 1i and 2j are the calculation nodes on particle 1 and particle 2, respectively

The linear motion of a particle can be calculated by Newton’s law of motion:

$$\boldsymbol{a}_1 = \boldsymbol{F}_1 / m_1 = \sum_{i=1}^{n} \boldsymbol{F}_{1i} / m_1, \tag{1}$$

where $\boldsymbol{a}_1$ is the linear acceleration of body 1; $\boldsymbol{F}_1$ is the summation of forces acting on body 1; n is the number of nodes on body 1; m_1 is the mass of body 1; and $\boldsymbol{F}_{1i}$ is the summation of forces acting on node 1i.

The rotational motion in Newton’s second law of motion in the model is expressed as

$$\boldsymbol{\alpha}_1 = \boldsymbol{\tau} / I_1 = \sum_{i=1}^{n} \boldsymbol{F}_{\mathrm{t}1i} \times \boldsymbol{d}_{1i0} / I_1, \tag{2}$$

where $\boldsymbol{\alpha}_1$ is the angular acceleration of body 1; I_1 is the principal moment of inertia; $\boldsymbol{\tau}$ is the torque impact on the body 1; $\boldsymbol{F}_{\mathrm{t}1i}$ is the tangential force acting on 1i; and $\boldsymbol{d}_{1i0}$ is the displacement vector from 1i to the center of mass.

3 Structure generation

3.1 Global shape of aggregate particle

To generate a particle assembly that corresponds to some actual mixtures, one first needs to characterize global shape. Once the shape has been described by a set of shape parameters, probability curves have to be provided for each parameter, so that it becomes possible to predict the probability of a certain shape (i.e., combination of shape parameters) in a mixture. Basically, HADES is designed to handle arbitrary shapes as long as the surface is tessellated by triangular or square surface elements of which the nodes are located on the surface. However, using real shapes for particles in packing simulations is too expensive and time-consuming. Therefore, choosing one or several shapes to represent different particles is more practical.

Generally, aggregate in concrete can be divided into two groups: gravel of fluvial origin and crushed rock, representing rounded and angular-shaped particles, respectively (Fig. 2). The ellipsoid was selected representing the river gravel particles. Conversely, the polyhedron is used for simulation of crushed rock grains (Fig. 2b). For efficient calculation in HADES, sufficient calculation nodes are necessary for every particle. Therefore, using a mesh is crucial for the generation of the particle. Ellipsoids are particularly interesting. A variety of shapes, ranging from oblate to oblong (Fig. 2), can be described with only three parameters.

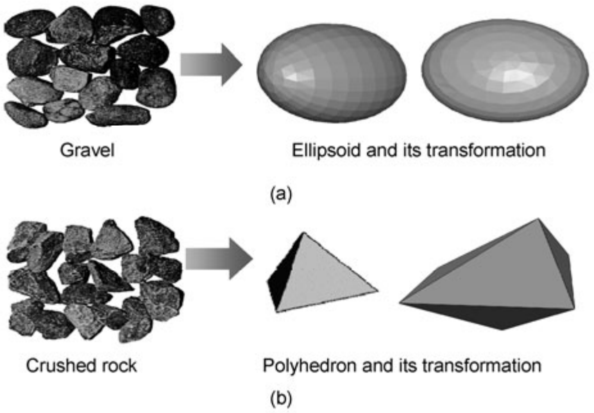


Fig. 2 Simulation strategy of arbitrary-shaped aggregate for river gravel (a) and crushed rock (b)

A specific group of shapes with 4–8 facetted surfaces are developed to represent practical crushed rock mixtures, following Guo (1988)'s field investigations. This greatly simplifies the simulation of crushed rock since only two parameters, i.e., the sieve size and maximum size of surface element, are required. Fig. 3 illustrates the particles with different numbers of facets and meshes. As stated above, polyhedron shapes are all regular. A more flexible method is developed for simulating more arbitrary-shaped particles. Quantitative image analysis is adopted to characterize particle shape by vertical and horizontal profiles of the aggregate. By combining the information of the two profiles using a 3D mesh program, the approximate shape of real aggregate can be reconstructed. Fig. 4 shows an application on an arbitrary-shaped aggregate (He *et al.*, 2009).

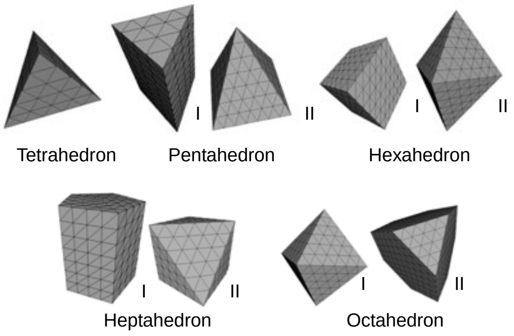


Fig. 3 Nine regular polyhedra with facet numbers of 4–8

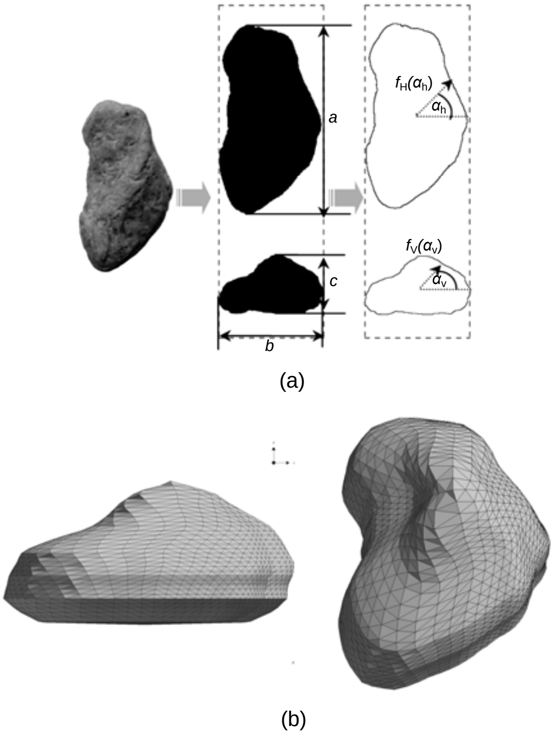


Fig. 4 Application on an arbitrary-shaped aggregate

(a) Characterization of shape information of a real aggregate by the image analysis method; (b) Two views of the reconstructed corresponding grain (He *et al.*, 2009). *a, b, c* represent the longest, median and shortest axes of a particle, respectively; $f_H(\alpha_h)$ and $f_V(\alpha_v)$ are the horizontal and vertical polar radii expressed as functions of the polar angles α_h and α_v, respectively

3.2 Global shape of cement particle

Garboczi and Bullard (2004) analyzed a standard reference cement, CCRL-133, with the Blaine fineness of about 350 m^2/kg. Synchrotron based X-ray imaging resolution was 0.95 μm per voxel. Clear images of cement particles were obtained after 3 h of hydration. It was also assumed that the obtained shape of the cement particles by X-ray micro-tomography (μCT) was close to the initial particles due to a small volume of cement that had been hydrated in their study (Garboczi and Bullard, 2004). Cement particles finer than 1 μm were not included in this study due to limited resolution. A spherical harmonic (SH) (Garboczi, 2002) analysis was applied for shape reconstruction and surface estimation. Results in terms of V (volume) and S (surface) provided an experimental database of cement, including some important parameters for cement hydration. The mutual regression line for the real cement particles is given by $S=8.0V^{0.64}$, with a correlation coefficient of 0.98. This curve is also given in Fig. 5a. Simulation by HADES was conducted with ellipsoidal and polyhedron particles. Both approaches gave a good simulation of the reference curve in Fig. 5. An example of the polyhedron-type particle simulation is shown in Fig. 5b (He, 2010).

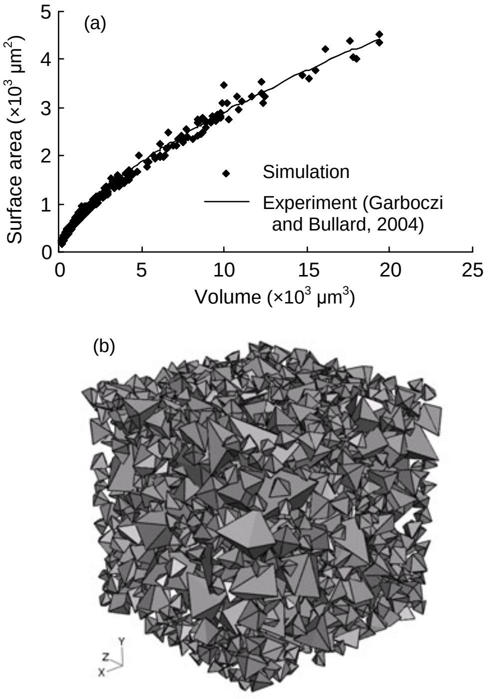


Fig. 5 Simulation of global shape of cement particles
(a) Experimental regression results (Garboczi and Bullard, 2004) and computer simulation of 1000 angular-shaped particles in 10–50 μm range; (b) A visualized model is displayed in loose random state (He, 2010)

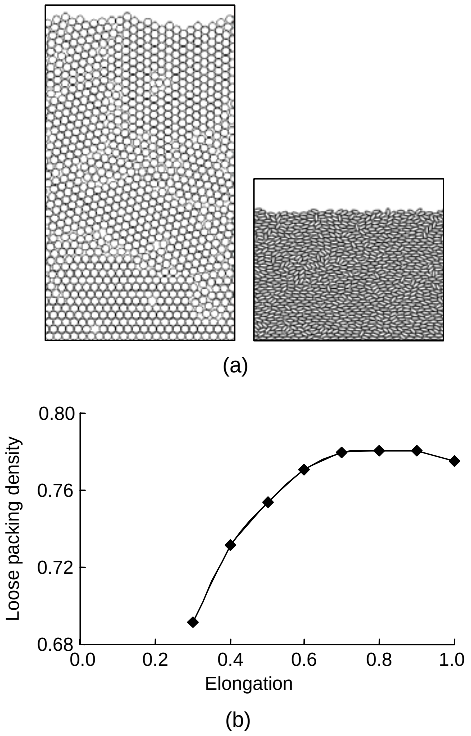
4 Exploration fields

4.1 Shape influence on particle packing

After a set of non-spherical particles is generated that approximates the actual mixture, the individual particles are positioned in a non-overlapping, but rather dilute way in some region or inside a container. This region can be defined by periodic boundaries, rigid boundaries or partly periodic and partly rigid boundaries (Stroeven and Guo, 2006). Each particle is given a random initial linear and angular velocity. Next, the particles are iteratively displaced to a position that is obtained by integrating the velocity over some (very small) time period. Similarly, the velocity of a particle at the next iteration, or time, is calculated by integrating the force (linear) or torque (angular) that acts on each particle. Currently, we have implemented gravitational forces, paste frictions and contact forces between particles.

Moreover, the boundaries, periodic or not, can be dynamically moved according to some user-defined functions. In this way, a number of experiments can be simulated. For example, by providing some sinusoidal motion of the container, shaking can be simulated, together with size segregation of the particles (under the influence of some gravitational force). Dense packing can be obtained in this way, but it is also possible to move the periodic or rigid walls of the container towards each other thereby increasing the volume density of the mixture. By measuring the force or stress that is exerted by the particles on these container walls, it is possible to decide when the "jammed state" is reached. Finally, the size of the samples (number of particles) is not predefined. This depends on the problem and the capacity of the computer.

Although it is difficult to find its physical representation, 2D mono-sized particle packing can be used for algorithm checks and for simple evaluation of shape effects. Loose packing of ellipses is simulated (Fig. 6). Here loose packing is defined as a packing of particles in the gravity field without employing shaking and compaction. To eliminate the influence of the container walls, periodic boundaries are applied at the lateral sides. 1000 mono-sized particles are used in each simulation. Elongation is used as the key shape index to generate ellipses. Elongation can be expressed as b/a, with a and b as the long and short axes of the ellipse, respectively. Eight types of ellipses with different elongation values ranging from 1.0 to 0.3 are selected in the packing trials, maintaining a constant ratio of the width of the container and a (approximately 23). The obtained random particle structures are displayed in Fig. 6, obviously revealing crystallization despite the periodic lateral boundaries (He, 2010). This is in agreement with Truskett *et al.* (1998) who found crystalline order to dominate systems of hard disks even at low packing fractions.



(a)

(b)

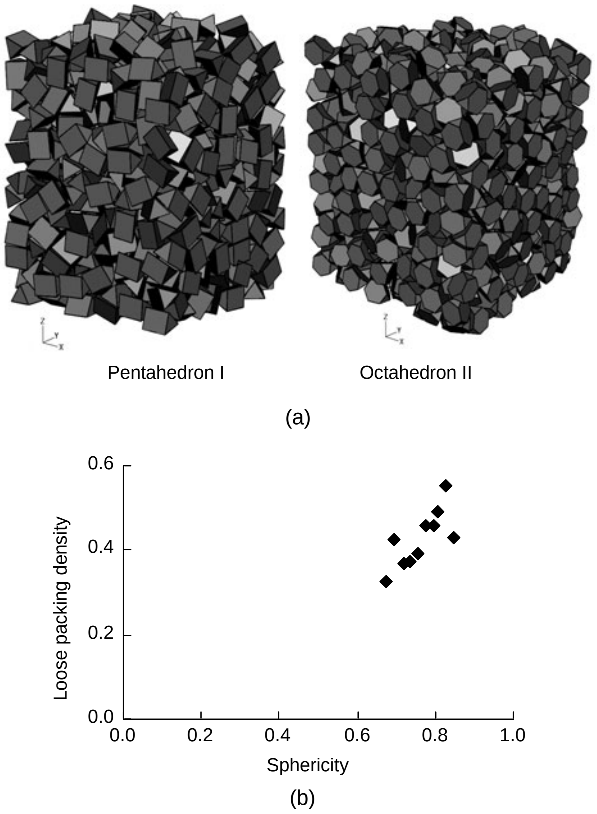
Fig. 6 Packing of 2D particles

(a) Two examples of loose packed structures of mono-sized ellipses for different elongation values; (b) Relationship of loose packing density (area fraction) with elongation (axes ratio)

A similar procedure is followed in the case of the 3D packing of mono-sized standard polyhedra of Fig. 3 (with facet numbers of 4 to 8). 864 particles with 10 mm sieve size were used for each simulation. Fig. 7a visually illustrates the loose packed structures with two typical shapes. Sphericity is defined as the surface area ratio of the equivalent sphere and particle (both having equal volume). As sphericity is a sensitive parameter for these shapes, loose packing density is presented in Fig. 7b as a function of sphericity.

4.2 Vibration effect on size segregation

Compaction by vibration applied during the production stage (in the construction industry as well as in the laboratory) has been demonstrated by SPACE augmenting the size segregation phenomenon due to the normal "wall effect". Assessment of influences exerted by global form and surface texture of aggregate on size segregation can be pursued by HADES system. This phenomenon is widely denoted as "Brazil nut effect (BNE)", and recognized as a relevant phenomenon in many branches of industry concerned with transport or vibration/shaking of particles (Stroeven *et al.*, 2007). The successive stills from a video in Fig. 8 reveal the 2D size segregation phenomenon arising from vertical vibration, i.e., the bigger elliptical grain moves to the top of the grain mixture. The situation is quite complicated and has received intense attention. Apart from the normal BNE, the reversed BNE is reported (Shinbrot, 2004), and even the horizontal BNE (Schnautz *et al.*, 2003). Relative densities and frequency details play a role, but the phenomenon is far from established, and some of the mechanisms are still speculative. According to Shinbrot (2004), we find ourselves facing the situation anticipated by Mark TWAIN "The researches of many commentators have already thrown much darkness on the subject, and it is probable that, if we continue we shall soon know nothing at all about it".



(a)

(b)

Fig. 7 Packing of 3D particles

(a) Random loose packing states of mono-sized particles with two typical shapes; (b) Random loose packing density as a function of sphericity of particles

Nevertheless, this may add to our studies on other consequences of particle size segregation phenomena as inflicted by rigid surfaces during compaction (mould on aggregates, and aggregate grains on cement particles). Cement particle size segregation in the fresh state finally leads, after hydration, to the evolution of a thin zone immediately neighbouring all the aggregate's surfaces of percolated porosity. Compaction by vibration yields an aggregate skeleton that governs the "nodes" in overlapping interfacial transition zones (ITZs) around the aggregate grains in which the percolated porosity layer is embedded. Such HADES multi-scale simulation will therefore be highly relevant with respect to durability issues (Stroeven *et al.*, 2008). It will be scientifically highly interesting and technologically extremely relevant to see whether and to what degree BNE will influence size segregation phenomena, of course depending on vibration characteristics and technological parameters, e.g., workability.

4.3 Workability testing

The methods for workability and compactability testing are numerous and highly uncorrelated. The methodology can be characterized by a large degree of pragmatism and a minor scientific basis. Specific solutions have been developed for sub-sectors of the concrete technology field, whereby simplicity under given conditions (either on-site or for laboratory testing) prevail. Some methods with overlapping fields of use have been compared as to ease of use, simplicity of equipment, and stability or reproducibility of outcomes. The "summary of concrete workability test methods" (Koehler and Fowler, 2003) offers a good survey.

Computer simulation would allow for an economic approach to such problems and could unify (at least partly) the methodology on fundamental issues. Compucrete is employed for that purpose, whereby the effect of the existing equipment on the compucrete can be simulated. Cementitious materials contain high amounts of aggregate, so particle interference will be a major mechanism governing workability of the mixture. Conventional RSA-based systems cannot (or, cannot economically) simulate particulate materials in this high-density range.

An election of the most promising methods has been simulated and outcomes mutually compared. Only a small number of current methods employ vibration, thereby better resembling workability during compaction. Vibration is necessary for workability testing of steel fibre reinforced concrete (SFRC) because of thixotropy. This situation will certainly be covered. Hence, the next step will be devoted to modelling the HADES configuration for the selected methodology approach, i.e., for performing tests in virtual reality. Fig. 9 shows an example of the HADES-simulated slump test, whereby

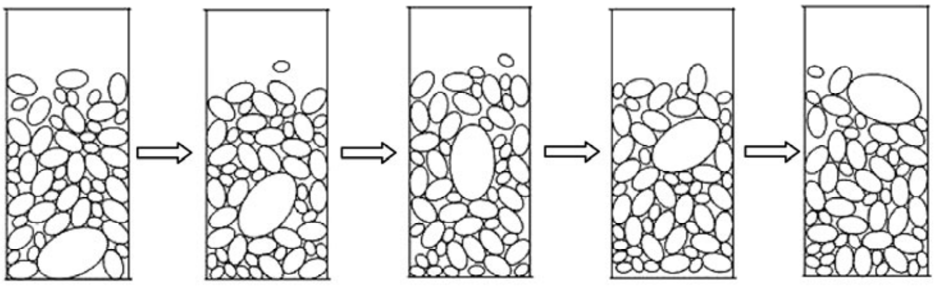


Fig. 8 Particle size segregation due to Brazil nut effect simulated by HADES in 2D

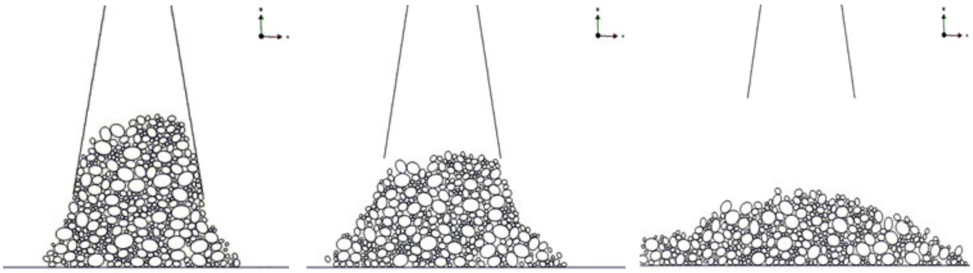


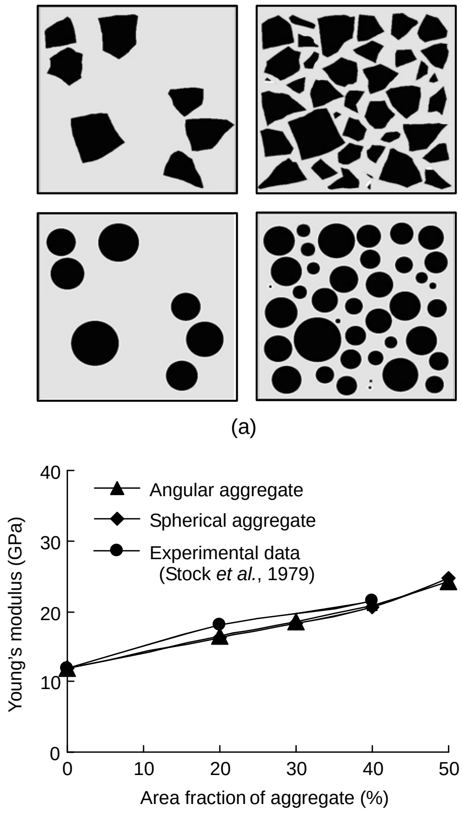
Fig. 9 Stages in the slump test (from left to right) as simulated by HADES

the average diameter of the fresh concrete mixture on the table surface is linked up with workability. Note that the effect of the cement paste matrix on the aggregate particles is simulated by adding inter-particle forces to the aggregate grains and by a coefficient that reflects the energy dissipation during aggregate grain movement. For details, please refer to (Stroeven, 1999).

4.4 Strength and damage estimation

HADES has been extended with the possibility of generating a (curved) surface with regularly structured FE mesh in which the material structure is explicitly modelled. Three components are distinguished: aggregates, cement matrix, and ITZs (the thin cement layer around each particle of which mechanical properties are different from those in bulk cement). These meshes can be constructed because HADES provides full descriptions of the material structure. Consequently, it is possible to provide the mesh generator with a function that defines the element size as a function of the distance to the nearest aggregate surfaces, for example. In this way, the ITZ—important for many mechanical properties in concrete—can be modelled with relatively small elements whilst the elements within aggregates can be much larger. For results pertaining to elastic and fracture properties of concrete, please refer to He (2010). Fig. 10 presents a simple example. Three-phase specimens containing simulated river aggregate and crushed rock, respectively, are considered. Sections of specimens in 2D with different amounts of equally dispersed aggregate are displayed in Fig. 10a. Shape effect on elastic properties is investigated on the basis of these three-phase concretes. ITZ is indicated by the proportionally thin white layer between aggregate (black) and matrix (grey). Fig. 10b reflects the observed influence of volume fraction and shape on Young's modulus. At the same volume fraction, the shape effect can be neglected in the normal concrete (He, 2010). Clearly, density in the compacted state will be different in both cases.

A parallel study focused on the fracture properties of these composites. An isotropic damage model (Jirásek and Marfia, 2005) (Fig. 11a) is applied for the description of the mechanical behavior of each concrete phase (He, 2010). In a direct tensile test, the peak force values of different 2D models are shown in Fig. 11b. Clearly, angularity promotes crack initiation and propagation, reducing ultimate tensile strength (He, 2010).



(a)

(b)

Fig. 10 Estimation of elastic properties of concrete with the meso-material models
(a) Two examples of meso-material models where different volume fractions (area fractions) and different shapes of aggregate (from top to bottom) were envisaged, respectively; dispersion in comparable cases is similar; (b) Young's modulus of concretes containing spherical or angular aggregate at different volume fractions; experimental data are due to Stock *et al.* (1979)

5 Discussion and conclusions

HADES allows investigation of hard core particle packing problems up to the jammed state inside and outside concrete technology whereby particles can be considered of arbitrary shape. Internal forces that govern the packing process can be emphasized. Particle systems that change their packing due to external static or dynamic forces (resulting in flow), and the inclusion of non-spherical shape that was shown to have an impact on density of the aggregate at the jammed state can be realized by the DEM system HADES. The system is used for exploration of the territories indicated herein.

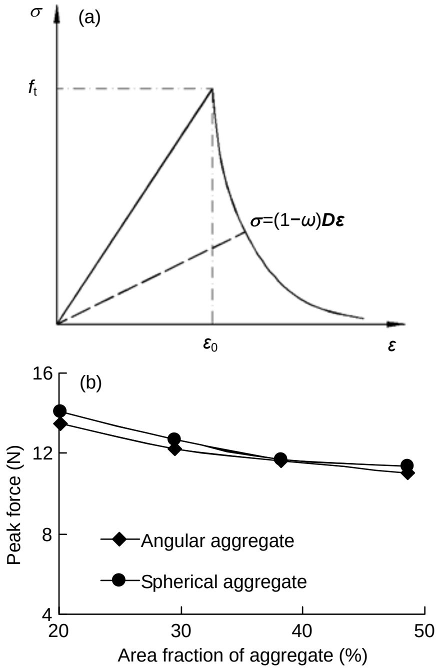


Fig. 11 Estimation of fracture properties of concrete with a damage model
(a) Stress-stain relationship in the damage model; (b) Ultimate tensile strength of models containing aggregate with different shapes at different volume fractions. σ and ε represent stress and strain of the material, respectively; $\boldsymbol{D}$ is the stiffness matrix of the undamaged material; ω is a damage scalar; and ε_0 and f_t are the strain at peak stress and the tensile strength, respectively

HADES (and earlier SPACE) can replace the traditional RSA computer simulation systems of the 20th century for exploration of the major mechanical and durability properties of concrete. It allows for tackling material optimization problems where particle packing is a major issue. Reliable information is offered on problems whereby particle dispersion is not Poisson-like, as in the particulate cementitious materials on different levels of its structure (aggregate on meso-level and cement and other binder blends on micro-level). Furthermore, the boundaries, periodic or not, can be dynamically moved according to some user-defined functions.

HADES incorporates arbitrary-shaped particles and force-based contacts. Particle shape involves global shape as well as surface texture. Particle sharp has influence on concrete's major properties (governing mechanical and durability performance). It also allows for simulation of effects of external forces on the particulate material.

References

Ansell, G.C., Dickinson, E., 1986. Sediment formation by Brownian dynamics simulation: effect of colloidal and hydrodynamic interaction on the sediment structure. *Journal of Chemical Physics*, **85**(7):4079-4086. [doi:10.1063/1.450879]

Ballani, F., 2005. A Case Study: Modeling of Self-Flowing Castables Based on Reconstructed 3D Images. 9th Euro Congress of Stereology and Image Analysis, Krakow, Poland, Polish Society of Stereology. Warsaw, Poland, p.282-288.

Bentz, D.P., Garboczi, E.J., Stutzman, P.E., 1993. Computer Modeling of the Interfacial Transition Zone in Concrete. *In*: Maso, J.C. (Ed.), Interfaces in Cementitious Composites, Taylor & Francis, New York, p.107-116.

Diamond, S., Thaulow, N., 2006. The patch microstructure in concrete: evidence that it exists and is not a backscatter SEM artifact. *Cement and Concrete Composites*, **28**(7): 606-612. [doi:10.1016/j.cemconcomp.2006.04.003]

Garboczi, E.J., 2002. Three-dimensional mathematical analysis of particle shape using X-ray tomography and spherical harmonics: Application to aggregates used in concrete. *Cement and Concrete Research*, **32**(10):1621-1638. [doi:10.1016/S0008-8846(02)00836-0]

Garboczi, E.J., Bullard, J.W., 2004. Shape analysis of reference cement. *Cement and Concrete Research*, **34**(10): 1933-1937. [doi:10.1016/j.cemconres.2004.01.006]

Guo, W., 1988. Some Material Parameters on Numerical Statistical Continuum Mechanics of Concrete. TU Delft Report: 25-88-38, Delft University of Technology, Delft, the Netherlands.

Guo, Z., Stroeven, M., Yang, W., Stroeven, P., 2007. Hades, Successor of Space System; Developments and New Territories for Exploration. 12th International Congress for Stereology, Saint Etienne, France.

He, H., 2010. Computational Modeling of Particle Packing in Concrete. PhD Thesis, Delft University of Technology, Delft, the Netherlands.

He, H., Stroeven, P., Guo, Z., Stroeven, M., 2008. Comparison of Experimental and SPACE Simulation Approaches to Particle Packing in Concrete. First International Conference on Microstructure Related Durability of Cementitious Composites, Nanjing, China. RILEM Publications S.A.R.L., Bagneux, France, p.1169-1178.

He, H., Guo, Z., Stroeven, P., Stroeven, M., Sluys, L.J., 2009. Characterization of the packing of aggregate in concrete by a discrete element approach. *Materials Characterization*, **60**(10):1082-1087. [doi:10.1016/j.matchar.2009.02.012]

Jirásek, M., Marfia, S., 2005. Non-local damage model based on displacement averaging. *International Journal for Numerical Methods in Engineering*, **63**(1):77-102. [doi:10.1002/nme.1262]

Jodrey, W.S., Tory, E.M., 1981. Computer simulation of isotropic, homogeneous, dense random packing of equal spheres. *Powder Technology*, **30**(2):111-118. [doi:10.1016/0032-5910(81)80003-4]

Klosek, J.T., 1997. The Integration of Fluid Dynamics with Discrete-Element Modeling Systems: Algorithms, Implementations and Applications. MS Thesis, Department of Civil and Environmental Engineering, MIT, Massachusetts, USA.

Koehler, E.P., Fowler, D.W., 2003. Summary of Concrete Workability Test Methods. Research Report ICAR 105-1, International Center for Aggregate Research, the University of Texas at Austin, Austin, TX. Available from http://www.icar.utexas.edu/publications/105/105_1.pdf [Accessed on Dec. 20, 2010]

Li, J.F., Yu, W.H., Chen, C.S., Yu, B.Y., Wei, W.C., 2006. Simulation of colloidal particle packing for photonic bandgap crystals. *Journal of the American Ceramic Society*, **89**(4):1257-1265. [doi:10.1111/j.1551-2916.2005.00889.x]

Markausas, D., Kačianauskas, R., 2006. Compacting of particles for biaxial compression test by discrete element method. *Journal of Civil Engineering and Management* **12**(2):153-161.

Meakawa, K., Chaube, R., Kishi, T., 1999. Modeling of Concrete Performance: Hydration, Micro-Structure Formation and Mass Transport. Taylor & Francis, New York.

Mościński, J., Bargieł, M., Rycerz, Z.A., Jacobs, P.W.M., 1989. The force-based algorithm for irregular close packing of equal spheres. *Molecular Simulation*, **3**(4):201-212. [doi:10.1080/08927028908031373]

O′Connor, R.M., Troczynski, J.R., Preece, D.S., Klosek, J.T., Williams, J.R., 1997. Discrete element modeling of sand production. *International Journal of Rock Mechanics and Mining Science*, **34**(3-4), No. 231, p.1-15. [doi:10.1016/S1365-1609(97)00198-6]

Puri, U.C., Uomoto, T., 2002. Characterization of distinct element modeling parameters for fresh concrete and its application in shotcrete simulations. *Journal of Materials in Civil Engineering*, **14**(2):137-144. [doi:10.1061/(ASCE)0899-1561(2002)14:2(137)]

Roelfstra, P.E., 1989. A Numerical Approach to Investigate the Properties of Numerical Concrete. PhD Thesis, Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland.

Schnautz, T., Brito, R., Kruelle, C.A., Rehberg, I., 2003. Horizontal Brazil-nut effect and its reverse. *Physical Review Letters*, **95**:028001. [doi:10.1103/PhysRevLett.95.028001]

Shinbrot, T., 2004. Granular materials: The Brazil nut effect—in reverse. *Nature*, **429**(6990):352-353. [doi:10.1038/429352b]

Stroeven, M., 1999. Discrete Numerical Modeling of Composite Materials—Application to Cementitious Materials. PhD Thesis, Delft University of Technology, Delft, the Netherlands.

Stroeven, P., 1973. Some Aspects of the Micro-Mechanics of Concrete. PhD Thesis, Delft University of Technology, Delft, the Netherlands.

Stroeven, P., Guo, Z., 2006. Modern routes to explore concrete's complex pore space. *Image Analysis Stereology*, **25**(2):75-85.

Stroeven, P., Sluys, L.J., Guo, Z., Stroeven, M., 2006. Virtual reality studies of concrete. *Forma*, **21**(3):227-242.

Stroeven, P., Sluys, L.J., Guo, Z., Stroeven, M., 2007. Does Brazil Nut Effect Influence Concrete Properties? Proceedings of 3rd International Symposium on Sustainability in Cement and Concrete, Istanbul, Turkey. Damla Matbaacilik Reklamcilik ve Yayincilik Tic., Ankara, Turkey.

Stroeven, P., He, H., Guo, Z., Stroeven, M., 2008. Pore Modelling Strategy in the Perspective of Concrete Durability. Proceedings of ICDCS Conference, Hangzhou, China. Zhejiang University Press, Hangzhou, China, p.493-499.

Stroeven, P., He, H., Guo, Z., Stroeven, M., 2009a. Particle packing in a model concrete at different levels of the microstructure: evidence of an intrinsic patchy nature. *Materials Characterization*, **60**(10):1088-1092. [doi:10.1016/j.matchar.2009.02.011]

Stroeven, P., Hu, J., Stroeven, M., 2009b. On the usefulness of discrete element computer modeling of particle packing for material characterization in concrete technology. *Computers and Concrete*, **6**(2):133-153.

Stroeven, P., Hu, J., Koleva, D.A., 2010. Concrete porosimetry: aspects of feasibility, reliability and economy. *Cement and Concrete Composites*, **32**(4):291-299. [doi:10.1016/j.cemconcomp.2010.01.007]

Truskett, T.M., Torquato, S., Sastry, S., Debenedetti, P.G., Stillinger, F.H., 1998. Structural precursor to freezing in the hard-disk and hard-sphere systems. *Physical Review E*, **58**(3):3083-3088. [doi:10.1103/PhysRevE.58.3083]

Tsunekawa, H., Iwashita, K., 2001. Numerical Simulation of Triaxial Test Using Two and Three Dimensional DEM. 4th International Conference on Micromechanics of Granular Media, Powder and Grains, Sendai, Japan. Balkema, Rotterdam, p.177-180.

van Breugel, K., 1991. Simulation of Hydration and Formation of Structure in Hardening Cement-Based Materials. PhD Thesis, Delft University of Technology, Delft, the Netherlands.

Williams, S.R., Philipse, A.P., 2003. Random packings of spheres and spherocylinders simulated by mechanical contraction. *Physical Review E*, **67**(1):051301. [doi:10.1103/PhysRevE.67.051301]

Wittmann, F.H., Roelfstra, P.E., Sadouki, H., 1985. Simulation and analysis of composition structures. *Materials Science and Engineering*, **68**(2):239-248. [doi:10.1016/0025-5416(85)90413-6]

Zaitsev, J.W., Wittmann, F.H., 1977. Crack Propagation in a Two-Phase Material Such as Concrete. International Conference on Fracture, ICF4, Waterloo, Canada. Pergamon, Oxford, UK, p.1197-1203.

Zheng, J.J., Guo, Z.Q., Pan, X.D., Stroeven, P., Sluys, L.J., 2010. ITZ volume fraction in concrete with spheroidal aggregate particles and application: Part I. Numerical algorithm. *Magazine of Concrete Research*, in press.