Computational Modelling of Particle Packing in Concrete
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Delft, October 2009
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<th>Description</th>
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<tr>
<td>2D</td>
<td>Two-Dimensional</td>
</tr>
<tr>
<td>3D</td>
<td>Three-Dimensional</td>
</tr>
<tr>
<td>ACN</td>
<td>Average Coordination Number</td>
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<tr>
<td>CAS</td>
<td>Concurrent Algorithm-based Simulation</td>
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<tr>
<td>CCD</td>
<td>Charge-Coupled Device</td>
</tr>
<tr>
<td>compucrete</td>
<td>COMPUTational conCRETE</td>
</tr>
<tr>
<td>CT</td>
<td>Computer Tomography</td>
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<tr>
<td>DEM</td>
<td>Discrete Element Method</td>
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<tr>
<td>DOH</td>
<td>Degree Of Hydration</td>
</tr>
<tr>
<td>FEM</td>
<td>Finite Element Method</td>
</tr>
<tr>
<td>HADES</td>
<td>HAbanera’s Discrete Element Simulator</td>
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<td>HPC</td>
<td>High Performance Concrete</td>
</tr>
<tr>
<td>IA</td>
<td>Image Analysis</td>
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<tr>
<td>ITZ</td>
<td>Interfacial Transition Zone</td>
</tr>
<tr>
<td>MC</td>
<td>Monte Carlo</td>
</tr>
<tr>
<td>NND</td>
<td>Nearest Neighbour Distance</td>
</tr>
<tr>
<td>NNSSS</td>
<td>Nearest Neighbour Surface-to-Surface Spacing</td>
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<tr>
<td>PC</td>
<td>Portland Cement</td>
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<tr>
<td>pdf</td>
<td>Probability Density Function</td>
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<tr>
<td>PRNG</td>
<td>Pseudo-Random Number Generator</td>
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<tr>
<td>PSD</td>
<td>Particle Size Distribution</td>
</tr>
<tr>
<td>RAE</td>
<td>Representative Area Element</td>
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<tr>
<td>realcrete</td>
<td>REAL conCRETE</td>
</tr>
<tr>
<td>RSA</td>
<td>Random Sequential Addition</td>
</tr>
<tr>
<td>RVE</td>
<td>Representative Volume Element</td>
</tr>
<tr>
<td>SCC</td>
<td>Self-Compacting Concrete</td>
</tr>
<tr>
<td>SH</td>
<td>Spherical Harmonic</td>
</tr>
<tr>
<td>SIA</td>
<td>Stereological Image Analysis</td>
</tr>
<tr>
<td>SPACE</td>
<td>Software Package for the Assessment of Compositional Evolution</td>
</tr>
<tr>
<td>UCN</td>
<td>Unhydrated Cement Nuclei</td>
</tr>
<tr>
<td>μCT</td>
<td>Micro-Computer Tomography</td>
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<tr>
<td>w/c</td>
<td>Water to Cement Ratio</td>
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CHAPTER 1

GENERAL INTRODUCTION

Particle packing is treated as an important topic by many concrete researchers, because of its relevance for materials properties. For the production of concrete a wide range of granular materials is required. Aggregate is used as concrete's skeleton, whereby the particles are stabilized by the cementitious matrix. Packing efficiency governs the spatial characteristics of this structure and thereby influences concrete's properties. Fine-grained sand can be used to further improve density of the aggregate structure for use in high performance concrete. The particulate cement is also frequently blended by fine mineral admixtures to influence performance of the paste and the properties of the matured concrete. The so-called filler effects increase packing density of the blended cement and possibly reduce water demand. High performance characteristics require suitable blending materials of proper fineness.

A number of theoretical packing models have been proposed for prediction of packing characteristics and the resulting concrete properties. A minimum voids ratio has been mathematically derived for certain particle size distributions. This allowed establishment of some optimum graded mixtures for concrete production. On the other hand, the computer simulation approach provides a powerful tool for simulating particle packing. Computational concrete (compucrete) has been developed for a wide range of research purposes. Application of computer simulation to particle packing offers a promising perspective in concrete technology; it provides a proper representation of the heterogeneous concrete material, and renders the possibility of studying the effects of a wide range of technological parameters.

In this chapter, a general introduction will be given to several relevant topics and the background will be sketched of this study on particle packing phenomena, cement blending in concrete, etc. Aims, study methodology and structure of this thesis will then be addressed in the second part of this chapter.

1.1 Overview

Particle packing phenomena are of relevance and acknowledged as highly important in various fields of technology. It has attracted the interest of scientists over many centuries. Many efforts have been made to attain maximum packing density or minimum void ratio. Shrinkage in sintering, fluid storage capacity, gas permeability and deformation in compaction are all depending on packing density (German, 1989). For storage of seeds, high packing densities are of economic relevance. Differential shrinkage stress can be developed due to different porosity (or packing density), leading to dry crack propagation in the finer ceramic processing (Franks and Lange, 1996).

In all these applications as well as in this thesis, a particle is defined as the smallest
discrete unit of a powder mass that can easily be separated from the rest. Particles can be of different nature, as to composition, size and shape. Size and shape predominantly influence packing. So, Fig. 1.1 shows two examples of particles having different size and shape and encountered in food engineering and nano-engineering, respectively.

As a typical composite material, concrete is composed of several granular materials and a hydraulic matrix. However, particulate nature of such cementitious materials extends to different structural levels and is not just limited to aggregate (gravel and sand) packing. Aggregate is packed into a mould to form the structure of concrete, while cement particles are “compacted” in water between aggregate grains. The packing phenomenon is therefore significant on meso-level as well as on micro-level for concrete. Particle packing details will directly affect the characteristics of concrete. High packing density of the aggregate can reduce the amount of binder and so the price of concrete. High packing density in binder can lead to denser microstructure, promoting high performance characteristics.

It is acknowledged that packing of granular material mainly depends on three parameters: size and shape of the particles and the way of packing (German, 1989). The impact on packing density of the first parameter has been widely investigated. Optimum and possible ranges of sieve curves have been recommended. Practical concepts have been incorporated in building codes. However, shape of aggregate has also been recognized for a long time to be important. But because of inherent complications in defining shape and in its experimental assessment, an explicit and universal approach is still missing. The packing method has been emphasized in practical construction conditions; enough vibration is recommended at appropriate workability levels.

Although a number of analytical packing models have been developed for density prediction, detailed information such as effects of packing method, shape impact as well as inhomogeneous packing structure, are still missing. An experimental approach to particle packing is time-consuming and laborious. Computer simulation of particle packing provides a promising alternative. The discrete element simulation method (DEM) in this study can take into consideration the size range and the shape of the particles as well as the packing method. Some applications will focus on the fresh packing of aggregate both on mono-sized
and multi-sized particles. Other applications of this modelling approach will focus on evaluating influences of particle packing on mechanical and microstructure properties of concrete.

1.2 Aims and research approaches

The study described in this thesis aims at developing a comprehensive model for discrete simulation of arbitrary-shaped particles and its application to a DEM-based packing system. Simulation strategies are proposed for arbitrary-shaped particles that resemble experimental approaches to particle shape. The simulation strategies are implemented into a DEM-based approach for particle packing. Influences exerted by particle shape, size and packing method are discussed in this study. One application of this model is to produce virtual concrete on meso-level. Taking advantages of the finite element method (FEM), influences of particle packing on mechanical properties of concrete are assessed. The effect of packing of cement particles on microstructure properties of cement paste are analyzed on micro-level. Self-healing capacity due to unhydrated cement is investigated by a DEM-based simulation system, whereby different cement types and packing densities are considered.

The discrete element simulation method constitutes the prime approach in this study. Image analysis and stereological estimation are additionally applied when necessary, such as for the reconstruction of 3D material structure. Continuum-based FEM is also used for property assessment of the virtual concrete.

1.3 Outline of research

Figure 1.2 presents an overview of the set up of this thesis that encompasses nine chapters. The main body of this thesis is divided into two parts: particle packing modelling and packing property assessment, on the one hand (Chapters 2-5), and packing-related mechanical properties of concrete and materials structure, on the other hand (Chapters 6-8).

Chapter 2 is dedicated to experimentally analyzing particle shape and to strategies for simulation of arbitrary-shaped particles. Different shape analysis methods for concrete particles are reviewed in this part. As an economic solution, the image analysis method is employed for shape analysis of a sample of real aggregate. Two different simulation strategies are proposed for the simulation of aggregate in concrete. A simulation strategy for cement grains is developed based on simple regular shapes, referring to published results obtained by X-ray tomography.

Chapter 3 is devoted to comparing different algorithms for simulation of particle packing. A traditional type of RSA system is developed and evaluated. Compared with a DEM-based packing system, the limitation and features of this approach are revealed. A possible improvement is applied to the traditional RSA system releasing somewhat the limitations imposed by this system. A possible application of RSA systems to arbitrary shaped particle packing is also discussed in this chapter.

Chapter 4 is concerned with the assessment of particle shape influences in 2D and 3D simulation approaches on packing characteristics using a DEM-based packing system. Some basic features of this system are highlighted in this part.

Chapter 5 presents analytical and numerical approaches to multi-sized particle packing. The contributions of finer particles to mono-sized packing are revealed by the mathematical
as well as the computational approach. Some wide-used mathematically optimum particle size distributions are discussed based on computer simulation results.

Chapter 6 and Chapter 7 deal with assessment of mechanical properties of numerical composite concrete by the DEM-based system. The influence of particle shape and particle packing density on elastic properties and fracture behaviour of concrete are discussed in this chapter. Additional effects of different parameters on mechanical properties of concrete are also considered.

In Chapter 8, a DEM-based cement packing and hydration system is used for investigating influences of particle packing on properties of the cement paste. The 3D material structures of models with different fineness of cement, different packing density (\(w/c\)) and different hydration conditions are evaluated by stereological methods. A sectional cracks and rehydration-based the healing model is proposed for assessment of self-healing capacity of concrete due to unhydrated cement.

Chapter 9 summarizes the findings and conclusions of this study, regarding the aims of this study, and presents some recommendations for the future research.

Fig. 1.2 Flowchart of this thesis
CHAPTER 2

EXPERIMENTAL ANALYSIS OF PARTICLE PACKING AND SHAPE SIMULATION

Aggregate occupies at least three-quarters of the volume of concrete, so its impact on concrete's properties is large. The sieve curve traditionally defines the aggregate size range. Another essential property is grain shape. Both, size and shape influence workability and the mechanical properties of concrete. The definition of the actual grain shape as well as the representation in a discrete element method (DEM) is complicated, however. Further, the real shape of aggregate or binder particles can vary widely. The sphere is therefore generally adopted in conventional simulation systems, despite imposing serious limitations. In this chapter, an experimental investigation of aggregate shape and particle packing, and a simulation strategy for the representation of arbitrary-shaped aggregate grains applied in concrete technology are presented. This simulation approach will be incorporated in a physical concurrent algorithm-based DEM system.

The shape of cement particles plays also an important role in the hydration process due to surface dissolution and the hardening process. Nevertheless, a spherical particle shape is normally assumed in conventional simulation systems, because of the inherent simplification in algorithm formulations and corresponding reduced computer time; however, at the cost of possibly biased simulation results. Recently, some reference cement was analyzed by X-ray micro-tomography. The results provide a real experimental database of this cement that yields valuable parameters for simulation of cement hydration. A shape analysis study was conducted with some simpler shape solutions, whereby the X-ray micro-tomography results served as a reference. Based on this analysis, a simulation strategy is proposed as a preferred approach to cement particle simulation. The generation of the densely packed microstructure of fresh cement paste can be further conducted by using an advanced DEM system.

2.1 Experimental approaches to shape analysis of particles

Aggregate is packed into a mould to format the structure of concrete. On the other hand, cement grains are also packed between the aggregate grains while in water. This phenomenon is more significant in lower water to cement ratio concrete, of course. Therefore, grain packing occurs in concrete both on meso-level as well as on micro-level. Hence, packing details will directly affect concrete's characteristics. Such details will mainly depend on three parameters: particle size and shape, and on packing method. The impact on packing density of the first parameter has been widely investigated. Possible ranges and even the optimum solution for sieve curves have been recommended. Practical concepts have been incorporated in building codes. Still, shape of
aggregate has also been recognized to be important for a long time. But because of inherent complications in defining shape and its experimental assessment, an explicit and universal approach is still missing. The packing method has been emphasized in practice by regulations in building codes; enough vibration is recommended at appropriate workability levels. Still, shape analysis is receiving more attention nowadays, because of its relevance. So far, several available methods have been employed for shape analysis of particles in concrete.

2.1.1 Manual measurements
Firstly, manual measurements for shape analysis have been developed for particle shape analysis, i.e., flatness (flakiness) and elongation indexes are obtained in this way. For instance, BE812, section 105.1 (1989) and BS 812, section 105.2 (1990) specify the manual method of measuring elongation and flatness of aggregate, as well as determination of the flakiness index CEN: EN933-3(6) (1997) part 3: determination of particle shape of aggregates and shape index CEN: EN933-4(7) (2008) part 4. A similar approach can also be found in ASTM standard (ASTM D4791) (1989), where elongation and flatness can be measured by a special designed calliper. But both measurement methods are laborious and time-consuming.

2.1.2 Image analysis (IA)
Image analysis (IA) pursues evaluating shape from 2-dimensional profiles. As a good approach to shape analysis, IA has been developed on the basis of improvements in optical and computer technology. It can provide more accurate and more elaborate results, replacing the major part of the aforementioned tedious manual approach (Janoo, 1998; Kwan et al., 1999a). Although the most work is on drawing out the three axes of aggregate by the method of image analysis, test approaches are very different. Kuo et al. (1996) placed the aggregate on the holder and produced images in two orthogonal directions. Another method of Maerz (2004) is putting the aggregation on the conveyor belt and imaging from the lying and standing position. It was assumed that the aggregate on the belt is in its stable position. Then, the thickness can be assessed from the side position. Prowell and Weingart (1999) analyzed the shape by putting a particle in a rotating cylinder and imaging the particle when it fell. This method assumes that the thickness of a particle is parallel to the rotating cylinder when it falls. Fernlund’s 3-D (Fernlund 1998; 2005) IA method is taking two images of a particle, lying and standing; both two pictures are used for the determination of the same index, width. Then length and thickness are correlated with the width, rendering the possibility of evaluation of size and shape. This constitutes a handy approach to assessment of shape and size. Rao et al. (2001) used three cameras to measure each aggregate particle from three orthogonal directions; the method is recognized as the University of Illinois Aggregate Image Analysis (UI-AIA). After application on ten aggregate samples, the analysis results were compared with traditional manual measurements for evaluation of this method. Kwan and his co-authors (1999a; 2000) used digital image processing to characterize shape of the 46 aggregate samples from five different sources. Different from other IA methods, Kwan et al. (1999a) used a new approach to estimate the volume and thickness of a particle. As a basic approach to shape analysis, they used it for identifying other shape indices. Determination of the packing density is also advocated by Kwan and Mora (2001). Packing density is analyzed with different shape indices. The promising relevancy of shape indices with packing density was determined by experiments of Kwan and Mora (2001).
2.1.3 Fourier analysis
Apart from direct linear dimensional image analysis, Fourier analysis is a mathematical way to achieve shape information from profiles of the aggregate, which can be achieved from images. Fourier analysis was used for more accurate shape identification, even involving surface texture (Wettimuny and Penumadu, 2004; Wang et al., 2005; Hu and Stroeven, 2006). In Fourier analysis, the boundary of an aggregate is expressed by (Wang et al. 2005):

\[ r(\theta) = r_0 + \sum_{i=1}^{\infty} (a_i \cos i\theta + b_i \sin i\theta) \]  

(2.1)

in which, \( r(\theta) \) is the radius of an edge point at angle \( \theta \); \( r_0 \) is average radius of particle, \( a_i \) and \( b_i \) are the amplitudes of the \( i \)th node in the Fourier expression; \( i \) represents the frequency.

Three different order parameters can be used to describe the shape, angularity and texture of a particle:

\[ \text{Shape (lumpiness): } \sum_{i=1}^{n_1} \sqrt{a_i^2 + b_i^2} \]  

(2.2)

\[ \text{Angularity (roughness): } \sum_{i=n_1+1}^{n_2} \sqrt{a_i^2 + b_i^2} \]  

(2.3)

\[ \text{Texture: } \sum_{i=n_2+1}^{n_3} \sqrt{a_i^2 + b_i^2} \]  

(2.4)

where, \( n_1 \), \( n_2 \) and \( n_3 \) are the three threshold frequencies to determine shape, angularity and surface texture. 8, 17 and 24 were adopted for \( n_1 \), \( n_2 \) and \( n_3 \), respectively, by Hu and Stroeven (2006).

2.1.4 Stereoscopic image analysis (SIA)
The IA method allows saving time and labour, as well as increasing the information about the aggregate character. However, the detailed 3-D shape properties may not be yielded from present Image analysis approach. The stereoscopic image analysis (SIA) method offers an alternative approach for this purpose. It is frequently used in microscopy approaches. It offers relevant information on shape in a more economic way as in traditional methods in vogue. The major application of SIA in the concrete field so far involves the reconstruction and subsequent analysis of fracture surfaces (Wu et al., 2000; Wang and Diamond, 2001; Nichols and Lange, 2006). Fig. 2.1 presents the set up of the proposed SIA for particle shape assessment. The matching of corresponding points in a pair of views will be performed by a reconstruction package MeX (Alicona GMBH, Austria). Surface information (i.e., depth, \( h \)) is calculated by (Broek, 1974; Tang et al., 2007):

\[ h = \frac{x_{\text{left}} - x_{\text{right}}}{2M \sin(\theta/2)} \]  

(2.5)

where, \( x_{\text{left}} \) and \( x_{\text{right}} \) are the coordinates of a corresponding point in the pair of images; \( M \) is
the magnification of the image; $\theta$ is the opening angle, shown in Fig. 2.1.

An example is illustrated here to show the potentials of SIA for aggregate shape reconstruction. Fig. 2.2 presents a pair of images of a crushed rock. The opening angle $\theta$ between two images is 10 degrees.

The pair of images was fed into the software MeX for 3D reconstruction, the projection of which is presented in Fig. 2.3. Some shape information can be obtained by the aforementioned software.

---

**Fig. 2.1 Schematic diagram of SIA of a particle**

**Fig. 2.2 Pair of views of a real particle by CCD cameras**

**Fig. 2.3 Reconstructed image in the SIA software MeX that is available for shape assessment**
Fig. 2.4 (a) A view of reconstructed surface point structure and (b) a view of reconstructed real shape of particle with surface mesh in GMSH

Furthermore, detailed information on the 3D reconstruction of the object in MeX can be transferred to other software packages for shape analysis, such as the mesh software GMSH (Geuzaine and Remacle, Webresource). The surface point structure produced by GMSH is shown in Fig. 2.4(a). Further, a surface mesh by triangles can be applied to the point structure. The result is plotted in Fig. 2.4(b).

The above example may demonstrate that SIA has its potentials for particle reconstruction. Compared with traditional IA methods and complex computer tomography method, advantages of SIA concern a more accurate and an elaborated particle reconstruction with simple equipment.

2.1.5 X-ray computer (micro-) tomography

As the shape of real particles in concrete is arbitrary and complicated, all information of shape can not be obtained by above approaches. Another technology, named X-ray computer tomography (micro-tomography) (CT or μCT), is employed (Garboczi, 2002; Garboczi and Bullard, 2004; Lin and Miller, 2005; Taylor et al., 2006). CT (μCT) is a non-destructive method for characterization of interior properties of opaque solids. It allows applying CT to characterize the shape of arbitrary particles (aggregate), especially in 3-D space (Garboczi, 2002).

Garboczi and Bullard (2004) analyzed a standard reference cement, CCRL-133, with Blaine fineness of about 350 m²/kg. Synchrotron based X-ray imaging resolution was 0.95 μm per voxel. Clear images of cement particles were obtained after 3 hours of hydration. It was also assumed that the obtained shape of cement particles by X-ray micro-tomography (μCT) was close to 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. The results provide an experimental database of cement, including some important parameters for cement hydration. Fig. 2.5(a) offers views on two typical cement particles. Fig. 2.5(b) shows S/V-data (correlation of surface area (S) and volume (V)) of reference cement particles and of spheres, differences being very obvious. The regression line for the real cement particles is given
by $S = 8.0V^{0.64}$, with a correlation coefficient of 0.98. $S = 4.84V^{2/3}$ for spheres. The surface area of cement particles is also size-dependent: larger grains have a lower coefficient of $V^{2/3}$, i.e. tending to a sphere.

2.1.6 Stereological method

Stereological methods are also applied to shape analysis, since they offer efficient tools to achieve high order information from low order profile information (Sahagian and Proussevitch, 1998; Hu and Stroeven, 2006). Different order shape indices, i.e. $s_1$, $s_2$ and $s_3$ are proposed based on stereological theory (Hu and Stroeven, 2006):

$$s_3 = \bar{V} / M_3(d), \quad s_2 = \bar{S} / M_2(d) \quad \text{and} \quad s_1 = \bar{L}_3 / M_1(d)$$

(2.6)

in which, $\bar{V}$ is the average volume of particles; $\bar{S}$ is the average surface area of particles; $\bar{L}_3$ is the average intercept length of particles; $M_3(d)$, $M_2(d)$ and $M_1(d)$ are moments of the size distribution function defined as:

$$M_n(d) = \frac{\sum_i d^n f_i(d)}{\sum_i f_i(d)}$$

(2.7)

in which $d$ is the size of a particle and $f_i(d)$ the probability density function. Compared with experimental results of different aggregate, higher order stereological shape index such as $s_3$ is more suitable for distinguishing and describe shape (Hu and Stroeven, 2006).

2.2 Shape analysis of a sample of real aggregate

Experimental shape analysis is conducted using the image analysis method. A sample of gravel from Stenvin Laboratory of Delft University of Technology with nominal size range
Fig. 2.6 Particle size distribution of aggregate samples on volume basis: (a) percentage distribution (b) cumulated percentage distribution

don from 8–16 mm was selected in this study. Size distribution was first defined by means of the sieve curve for three different samples, using standard sieve size of 6.3, 8, 11.2, 16 and 19 mm. Final particle size distributions (PSD) are plotted in Fig. 2.6. It shows around 5% of aggregate are smaller than nominal lower bound (8 mm), while 5% of gravel are larger than nominal upper bound (16 mm).

196 gravel grains actually ranging from 11.2–16 mm were randomly selected from the samples and applied to image analysis. Horizontal and vertical projection images were made of each particle with its suitable position. The binary horizontal projection image is shown in Fig. 2.7. Image analysis software, ImageJ (freely downloadable from the National Institutes of Health, Washington DC, USA, [http://rsb.info.nih.gov/ij](http://rsb.info.nih.gov/ij)) was used for assessment of reliable shape information.

Three axes per particle are distinguished by the IA method, whereby a, b, c represent the longest, median and shortest axis of a particle, shown in Fig. 2.8. Distributions of the values of the length of the respective axes are presented in Fig. 2.9(a). It shows values pertaining to the respective axes to be distributed in scatter band on different size levels. Cumulated PSDs of the three axes are displayed in Fig. 2.9(b), revealing somewhat different shapes in this

![Binary horizontal projected image of 196 gravel grains](image-url)
Fig. 2.8 *Three axes assessment by IA of the orthogonal projection images of a particle*

(a) Length distribution and (b) cumulated length distribution of the three axes distinguished in the orthogonal projection images of 196 aggregate particles.

Sample. Part of the values of the shortest axis is falling below the lower bound of the sieve range (11.2 mm), whereas part of the values of the longest axis exceeds the upper bound value of the sieve range (16 mm). The values of the median axis roughly correspond to the sieve range. Average values of the three axes of these 196 particle projections are 9.2, 13.2 and 18.1 mm, respectively. Therefore, the longest axis of the projected particle can exceed the largest sieve size, such as in case of elongated particles (Kwan *et al.*, 1999a). In other words, sieve measurements of a particle sample largely depend on information on *b* and *c*. More specifically, information on the median axis is particularly correlated with sieve size data.

Other shape indices can be derived from the system of three principle axes of the projection images. For instance, elongation is defined by *b/a*, and flatness by *c/b*. As shape factor Janoo (1998) has proposed:

\[
\text{Shape factor} = \frac{ac}{b^2} \tag{2.8}
\]

Additionally, sphericity is defined as the ratio of the surface area of an equivalent sphere to that of the particle (both having the same volume). To avoid determination of surface area, sphericity is simplified as (Janoo, 1998):
Experimental Analysis of Particle Packing and Shape Simulation

\[ \text{Sphericity} = \frac{12.8 \sqrt{\frac{c^2}{ab}}}{1 + \frac{(a+b)c}{ab} + 6 \left[ 1 + \frac{c^2(a^2+b^2)}{a^2b^2} \right]} \]  

(2.9)

Distributions of elongation and flatness values are plotted in Fig. 2.10. Obviously, the majority of the particles are neither very elongated nor flat, since elongation and flatness are exceeding 0.5. These values are in agreement with ASTM D 2488-90 (1996) criterion for identification of particle flatness and elongation (both 0.3). But the distributions of two shape parameters are widely (randomly) scattered. Average elongation and flatness are 0.75 and 0.68, respectively. These results can be used as references in aggregate simulation.

The results of shape factor and sphericity of 196 particles are presented in Fig. 2.11. The average shape factor is 1.0, which seems pointing toward a rounded or cubic particle shape. The distribution of shape factors (in Fig. 2.11(a)) reveals many particles to be elongated (shape factor < 1.0), while other particles seem blade-shaped (shape factor > 1.0). The majority of sphericity values of particles are higher than 0.8. The average sphericity is 0.87.

Barksdale and Itani (1994) used the combination of shape factor and sphericity to classify aggregate as disc, equidimensional, blade and rod. The description of each type (Lees, 1964; Barksdale and Itani, 1994; Janoo, 1998) is shown in Table 2.1. Furthermore, Barksdale and Itani (1994) developed a chart to identify the aggregate type, shown in Fig. 2.12. Some experimental results obtained on different types of aggregate by Barksdale and Itani (1994) are also listed in Fig. 2.12, where \( F \) is shape factor and \( \Psi \) refers to sphericity. The average experimental results of this aggregate are also listed in the figure. It shows the results obtained on the 196 gravel particles to be close to those of Barksdale and Itani. Generally, gravel from fluvial origin has approximately equidimensional proportions. However, crushed rock aggregate tends to a blade-like shape and the level seems depended on the type of aggregate.

![Fig. 2.10](image_url) (a) Elongation and (b) flatness distributions of 196 particles
Loose packing evaluation was then conducted with various samples based on different sieve size ranges. A standard slump cone is used as the container, the size of which is well known. The slump cone is filled with the successive samples until its maximum capacity, without employing shaking or vibration. The filling process is only affected by gravity (see Fig. 2.13(a)). For another application of such measurements for workability testing from which Fig. 2.13(b) is selected, see (Guo et al., 2009). The weight of each batch of aggregate loosely packed inside the slump cone is recorded. The volume of each batch of aggregate was estimated by the drainage method. Final results are shown in Table 2.2. The average of loose packing density of each batch of gravel is about 0.53.

Table 2.1 Description of aggregate type from combination of shape factor and sphericity

<table>
<thead>
<tr>
<th>Shape</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Disc</td>
<td>Slabby in appearance, but not elongated</td>
</tr>
<tr>
<td>Equidimensional</td>
<td>Neither slabby appearance nor elongated</td>
</tr>
<tr>
<td>Blade</td>
<td>Slabby appearance</td>
</tr>
<tr>
<td>Rod</td>
<td>Elongated, but not slabby in appearance</td>
</tr>
</tbody>
</table>

![Fig. 2.11](image) (a) Shape factor and (b) sphericity distributions of 196 particles

![Fig. 2.12](image) Shape classification of aggregate by shape factor and sphericity (some results taken from Barksdale and Itani, 1994)
2.3 Shape simulation of aggregate

A particle is defined as the smallest discrete unit of a powder mass that cannot be easily subdivided (German, 1989). The shapes of real particles are irregular, either from coarse aggregate or from mineral admixture. Using real shapes for particles in packing simulations is too expensive and (computer) time-consuming. In other words, it is not practical to model a large number of particles, each with its actual shape and size (Thomas and Bray, 1999). Therefore, choosing one or several shapes to represent different particles is a more practical way. Different simulation methods can be adopted for simulation of aggregate.

2.3.1 Origin based simplified method

Generally, aggregate in concrete can be divided into two groups: gravel of fluvial origin and crushed rock, representing rounded and angular-shaped particles, respectively, as shown in Fig. 2.14(a). The ellipsoid was selected to represent the gravel particles. On the contrary, the polyhedron was used for simulation of crushed rock grains, also shown in Fig. 2.14(a). For efficiency of calculation in an DEM, enough calculation nodes are necessary for every particle. Therefore, using a mesh is crucial for the generation of the particle.

Ellipsoids are particularly interesting because with only 3 parameters a variety of shapes, ranging from oblate to oblong can be described, as shown in Fig. 2.14(b) (i-iii). Two extra parameters are introduced that allow a range of differently-shaped particles derived from the ellipsoids, namely, maximum size of surface element and maximum angle between the normal vectors to neighbouring surface elements at a node. These parameters control how much the surface mesh follows the actual mathematical shape.

**Table 2.2 Physical properties of the specimens in different range used in the study**

<table>
<thead>
<tr>
<th>Sieve size range</th>
<th>8–11.2 (mm)</th>
<th>11.2–16 (mm)</th>
<th>8–16 (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass (kg)</td>
<td>7.860</td>
<td>7.775</td>
<td>7.830</td>
</tr>
<tr>
<td>Volume (l)</td>
<td>3.05</td>
<td>2.933</td>
<td>2.81</td>
</tr>
<tr>
<td>Absolute Density (10^3kg/m³)</td>
<td>2.577</td>
<td>2.651</td>
<td>2.786</td>
</tr>
<tr>
<td>Loose packing density</td>
<td>0.555</td>
<td>0.534</td>
<td>0.511</td>
</tr>
</tbody>
</table>
A specific group of shapes with 4-8 faceted surfaces are developed to represent the crushed rock, following Guo's field investigations (Guo, 1988). This greatly simplifies the simulation of crushed rock since only the two parameters, i.e. sieve size and the maximum size of surface element, are required. Table 2.3 illustrates the particles with different number of facets and meshes. The quantity proportions of each polyhedron in the whole group of simulated crush rock proposed by Guo (1988) are also revealed in Table 2.3.

As stated above, polyhedron shapes are all regular. A method is developed for simulating more arbitrary-shaped crushed rock particles. The 8 faceted octahedron is selected to represent the basic shape of crushed rock, based on the conclusion that no more than 8 facets were found in normal crushed rock samples (Guo, 1988). An arbitrary octahedron could be realized by specification of parameters as given in Fig. 2.15(a). After generating the basic shape of the arbitrary octahedron, the mesh is applied to the surface of the grain (see Fig. 2.15(b)).

Table 2.3 Multi-faceted regular polyhedrons with different mesh systems

<table>
<thead>
<tr>
<th>Tetrahedron</th>
<th>Pentahedron</th>
<th>Hexahedron</th>
<th>Heptahedron</th>
<th>Octahedron</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 facets</td>
<td>5 facets</td>
<td>6 facets</td>
<td>7 facets</td>
<td>8 facets</td>
</tr>
<tr>
<td>10%</td>
<td>25%</td>
<td>35%</td>
<td>20%</td>
<td>10%</td>
</tr>
</tbody>
</table>

Fig. 2.14 (a) Simulation strategy of arbitrary shaped aggregate; (b) Differently shaped ellipsoids: lengths of the three semi-axes are 6, 8, 10 in (i), 5, 15, 22 in (ii) and 4, 5, 16 in (iii)
To simulate the surface texture of aggregate grains, a more explicit generation method was applied, i.e. a sine function was chosen for adjusting positions of surface nodes, viz. Eq. (2.10).

\begin{align}
    x_i &= (1 + A_0 \sin \theta_i)x_{i0} \\
    y_i &= (1 + A_0 \sin \theta_i)y_{i0} \\
    z_i &= (1 + A_0 \sin \theta_i)z_{i0}
\end{align} \tag{2.10}

By keeping $x_i/x_{i0} = y_i/y_{i0} = z_i/z_{i0} = (1 + A_0 \sin \theta_i)$, the nodes can be readjusted on the line between original positions and origin. $x_{i0}, y_{i0}, z_{i0}$ and $x_i, y_i, z_i$ are coordinates of a node on the surface before and after the adjustment, respectively. $A_0$ is the vibration magnitude. $\theta_i = \theta_{i-1} + d\theta$ is the phase angle. Different surface textures can be generated in this way as shown in Table 2.4.

Table 2.4 Surface texture simulation of an arbitrary octahedron with different parameters

<table>
<thead>
<tr>
<th>$d\theta$</th>
<th>$A_0$</th>
<th>0.01</th>
<th>0.03</th>
<th>0.05</th>
<th>0.10</th>
</tr>
</thead>
<tbody>
<tr>
<td>30°</td>
<td></td>
<td><img src="image1.png" alt="Image" /></td>
<td><img src="image2.png" alt="Image" /></td>
<td><img src="image3.png" alt="Image" /></td>
<td><img src="image4.png" alt="Image" /></td>
</tr>
<tr>
<td>60°</td>
<td></td>
<td><img src="image5.png" alt="Image" /></td>
<td><img src="image6.png" alt="Image" /></td>
<td><img src="image7.png" alt="Image" /></td>
<td><img src="image8.png" alt="Image" /></td>
</tr>
<tr>
<td>90°</td>
<td></td>
<td><img src="image9.png" alt="Image" /></td>
<td><img src="image10.png" alt="Image" /></td>
<td><img src="image11.png" alt="Image" /></td>
<td><img src="image12.png" alt="Image" /></td>
</tr>
</tbody>
</table>
2.3.2 Flexible simulation method

The method stated above is a simplified regular shape simulation strategy for different types of aggregate. Here a more flexible method is presented applicable in 2D as well as 3D space.

In general, 2D particle packing simulation has the advantage of promoting simplicity and reducing calculation time. Hence, 2D arbitrary shape simulation is definitely attractive. Particle boundaries to define shape in 2D can be characterized by polar coordinates. As important form or shape parameters, particle length \( a \) and breadth \( b \) in 2D, and length \( a \), breadth \( b \) and thickness \( c \) in 3D are frequently used. Some other shape parameters can be derived from these three indices such as elongation, flatness (flakiness), shape factor and sphericity (Janoo, 1998; Hayakawa and Oguchi, 2005; Stroeven et al., 2009a). Therefore, it is important to keep forms \((a, b, c)\) as the control parameters in simulation.

An arbitrary 2D shape in Fig. 2.16(a) can be expressed by its polar coordinates:

\[
r = f(\alpha) = f_{AB}(\alpha) + f_{BC}(\alpha) + f_{CD}(\alpha) + f_{DA}(\alpha)
\]

where, polar radius \( r \) is expressed as function of polar angle \( \alpha \), which can be divided into four value ranges by form vertices A, B, C, and D.

Any suitable expression of \( f(\alpha) \) between form vertices and inner angle between long axis and short axis \( \theta \) can be applied to simulate a 2D shape. For instance, Beddow and Meloy’s morphological law can be applied to generate rounded particles (Beddow and Meloy, 1980; Wittmann et al., 1984; Wang et al., 1999) see equation (2.12). Some typical 2D shape can be achieved by this flexible method, illustrated in Fig. 2.16(b).

\[
\log(r_i / r_0) = -p \cdot \log(i) - b
\]

in which, \( r_i \) is the amplitude of the \( ith \) node in Fourier expression; \( r_0 \) is average radius of particle, \( r = r_0 + \sum r_i \cos(i\alpha + \theta_i) \) (\( \theta_i \) and \( \alpha \) are the phase angle and polar angle, respectively); \( p \) and \( b \) are the shape related parameters.

Compared with 2D shape simulation, reconstruction of 3D shape is more complex. One more sophisticated and direct way is using X-ray tomography and spherical harmonics.

Fig.2.16 (a) Characterization of 2D shape with polar coordinates; (b) some reconstructed typical 2D shape examples
(Garboczi, 2002). But it is still time-consuming and requires sophisticated equipment. A more realistic simulation approach uses more popular equipment to capture major shape information of particles. Quantitative image analysis is a widely used method to characterize particle shape. By this method, vertical and horizontal profiles of the aggregate in Fig. 2.17 can be captured. Next, the profile boundaries can be discretized into polar coordinates (vertical $f_v(\alpha)$ and horizontal $f_h(\alpha)$) and stored into a database.

By combining the information of two profiles by a 3D mesh program, the rough shape of real aggregate of Fig. 2.17 can be reconstructed (Fig. 2.18). Of course, different fineness of mesh will guarantee different precision of shape reconstruction, which is illustrated in Fig. 2.18. In the case no detailed experimental profile data is available, flexible shape can be achieved by specification of the profile equations $f_v(\alpha)$ and $f_h(\alpha)$. The earlier mentioned three form factors are used as the control information for reconstructing a 3D shape in a way similar as explained for the 2D case. Some examples of 3D shape simulation are presented in Figs. 2.19.

---

**Fig. 2.17** Characterization of shape information of a real aggregate by image analysis method

**Fig. 2.18** Two views of reconstruction the grain in Fig. 2.17 with (a) fine 3D mesh and (b) course 3D mesh, respectively.
2.4 Shape simulation of cement grains

2.4.1 Introduction
Concrete is made of hard inclusions surrounded by a hydraulic, cementitious matrix. Bonding between aggregate and hardened matrix provides concrete with a capacity to resist tensile stresses. Properties of the cement paste in addition to mixture design and curing condition control the mechanical behaviour of concrete. The shape of cement particles plays also an important role in the hydration process and structure formation, including pore space. Cement hydration in a DEM approach renders the possibility of investigating microstructure development and properties of concrete. A digital image-based model (Bentz, 1997) as well as continuum models (van Breugel, 1997; Navi and Pignat, 1999; Stroeven, 1999) have been developed for this purpose. Apart from the digital-image-based model, particle shape is generally assumed spherical in such systems, because of inherent simplification in algorithm formulation; however, at the cost of possibly biased simulation results.

Computer X-ray micro-tomography offers a potential solution for shape assessment of cements, as shown by Garboczi and Bullard (2004) and by Bullard and Garboczi (2006). The microstructures of hydrated cements based on actual grain shape and on spherical shape were found significantly different in this study. The results provide an experimental database of this cement that yields some valuable parameters for DEM simulation of cement hydration.

Using grains in numerical simulation similar to the real ones would be too expensive. So, it is crucial finding simpler shapes that are sufficiently representative. A shape analysis study was therefore conducted with some simpler shapes. Based on this analysis, a simulation strategy is proposed for cement. Implementation of this simulation strategy in the concurrent-algorithm based particle packing simulation system HADES (HAbanera’s Discrete Element Simulator) and some packing simulations are also discussed in this section.

2.4.2 Shape Analysis
The spherical grain shape is commonly adopted in conventional cement hydration simulation systems (van Breugel, 1997; Navi and Pignat 1999; Stroeven, 1999). However, the aforementioned experiments by X-ray micro-tomography have shown that this is a somewhat biased approach. More realistic but still cost-effective particle shapes should therefore be implemented in DEM systems.
2.4.2.1 Analysis of some polyhedra

The polyhedron is a potentially promising choice for particle shape. Nine polyhedra with facet numbers from 4 to 8 are selected in this preliminary shape analysis (see, Fig. 2.20). As the surface-to-volume \((S/V)\) relationship was the most important information obtained from the experimental reference, values of these shape indices are listed in Table 2.5 and plotted in Fig. 2.21. Sphericity is defined as surface area ratio of sphere and particle (both have similar volume). The surface over volume \(S/V\)-relationship can generally be expressed by \(S = aV^{2/3}\) \((a\) is a coefficient). Within effective experimental volume range of 10,000–150,000 \(\mu m^3\) (Garboczi and Bullard, 2004), coefficient \(a = 5.8\) was found by regression analysis, with a coefficient of variation lower than 5%. Proposed shapes should therefore approximate this value. In this case, sphericity can be calculated by:

\[
\text{Sphericity} = \frac{S_{\text{eq, sphere}}}{S_{\text{particle}}} = \frac{4\pi \left(\frac{3V}{4\pi}\right)^{2/3}}{aV^{2/3}} \approx 0.83
\]  
(2.13)

Fig. 2.20 Nine regular polyhedra with facet number 4~8

![Nine regular polyhedra with facet number 4~8](image)

Fig. 2.21 Surface area versus volume curves of reference cement and some regular polyhedra

![Surface area versus volume curves](image)
Table 2.5 Comparison of shape indices of regular polyhedra and spheres (S: surface area, V: volume)

<table>
<thead>
<tr>
<th>Shapes</th>
<th>Facet number</th>
<th>Sphericity</th>
<th>$S/V^{2/3}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tetrahedron</td>
<td>4</td>
<td>0.67</td>
<td>7.21</td>
</tr>
<tr>
<td>Pentahedron I</td>
<td>5</td>
<td>0.70</td>
<td>6.95</td>
</tr>
<tr>
<td>Pentahedron II</td>
<td>5</td>
<td>0.72</td>
<td>6.71</td>
</tr>
<tr>
<td>Hexahedron</td>
<td>6</td>
<td>0.76</td>
<td>6.39</td>
</tr>
<tr>
<td>Cube</td>
<td>6</td>
<td>0.81</td>
<td>6.00</td>
</tr>
<tr>
<td>Heptahedron I</td>
<td>7</td>
<td>0.83</td>
<td>5.83</td>
</tr>
<tr>
<td>Heptahedron II</td>
<td>7</td>
<td>0.80</td>
<td>6.06</td>
</tr>
<tr>
<td>Octahedron I</td>
<td>8</td>
<td>0.85</td>
<td>5.72</td>
</tr>
<tr>
<td>Octahedron II</td>
<td>8</td>
<td>0.78</td>
<td>6.24</td>
</tr>
<tr>
<td>Sphere</td>
<td>∞</td>
<td>1.00</td>
<td>4.84</td>
</tr>
</tbody>
</table>

From Table 2.5 and Fig. 2.21, it is concluded that the heptahedron I and the octahedron I offer the most promising solutions. The octahedron is selected for simulation study because of allowing an easier transformation into irregular shapes by parameter variation. Three axes can be employed for this purpose, as in He et al. (2008b). Since the $S/V$-curve of an octahedron is close to that of reference cement, some limited random variation can be applied for the diversity of particle shape.

2.4.2.2 Analysis of ellipsoids

Ellipsoids offer another promising possibility. Moreover, this shape can be easily derived from a sphere. Three principal axes ($a$ represents longest, $b$ medium size and $c$ shortest axis, as shown in Fig. 2.22.) determine the shape of an ellipsoid. By parameter variation, different ellipsoids with different $S/V$-relationships can be derived. $V$ and $S$ can be obtained by (Weisstein, Websource):

$$V = \frac{4}{3} \pi abc$$

$$S = 2b\sqrt{2}\int_0^a \sqrt{a^2 + c^2 + (a^2 - c^2) \cos(2\phi) \sin \phi}$$

$$\times E\left[\frac{c}{b} \sqrt{\frac{2(b^2 - a^2)}{a^2 + c^2 + (a^2 - c^2) \cos(2\phi) \sin \phi}} \sin \phi\right] d\phi$$

Fig. 2.22 An ellipsoid with three axes: $a, b, c$
in which, \( E = (b^2 \cos^2 \theta + a^2 \sin^2 \theta) \sin^2 \phi \) is a coefficient of the first fundamental form; \( \phi \) is a polar angle.

Flatness and elongation are defined as \( c/a \) and \( b/a \), respectively. So, the distribution contours of sphericity with different elongation and flatness values can be constructed (see, Fig. 2.23).

Because \( c < b < a \), elongation is always exceeding flatness. Fig. 2.23(a) reveals that if elongation and flatness are both larger than 0.5, sphericity of an ellipsoid will be close to 1. \( S/V^{2/3} \)-contours with elongation and flatness are plotted in Fig. 2.23(b). The hatched region can be selected as optimum solution.

### 2.4.3 Implementation of the selected shapes in DEM

Modern high performance concretes are produced at low water to cement ratio: volume content of the cement in the paste may be as high as 60%. The traditional DEM simulation system in concrete technology is using random generators to disperse cement (and mineral admixture) particles on micro-level in the watery environment during the fresh state. These systems are referred to as random sequential (particle) addition (RSA) systems. As stipulated elsewhere, they generate particle packing distinct from actual ones (Stroeven et al., 2008). Additionally, RSA systems cannot produce high densities. Concurrent algorithm-based simulation (CAS) systems were developed starting from RSA procedures, avoiding such limitations (Stroeven, 1999; Williams and Philipse, 2003; Stroeven et al., 2009b). An advanced CAS system like HADES has been developed with capabilities of packing arbitrary shaped particles (He et al., 2008a). The preferred shapes defined in this study can also be incorporated in HADES. After assessment of grain shape, mass properties are assigned to each particle, e.g., mass, centre of mass, moment of inertia. Some packing simulation examples are presented in Chapter 4.

Figure 2.24(a) illustrates S-V information of a group of simulated cement grains using flat
ellipsoids, which fits experimental results (Garboczi and Bullard, 2004) well. A visualized structure of correspondingly loose packed ellipsoids obtained by HADES is plotted in Fig. 2.24(b).

Figure 2.25 shows two S/V-distributions of two randomly generated octahedron examples with an experimental reference curve. Fig. 2.25(a) reveals the case of 1000 particles with longest axis in 10–50 μm size range. The S/V-relationship complies well with experiments. But in the case of the larger particles in Fig. 2.25(b) (maximum longest axis of particles is around 100 μm), the simulated particles have a slightly higher surface area compared with the experimental reference case. It indicates that larger particles tend to a spherical shape. One possible reason for this phenomenon is that those larger particles are to a smaller degree affected by grinding and thus less angular as a result.

Figure 2.26(a) shows an example of a packed structure of arbitrary octahedrons and a section image in Fig. 2.26(b). A packed structure of simulated cement particles with non-spherical shape can be used as a fresh cement paste structure.
Fig. 2.26 (a) Visualized structure of compacted grains and (b) section of the simulated structure (1000 octahedron grains in 10–50 μm range)

To select the more reasonable shapes for simulation of cement particle grains, a review will focus on the production process of cement. Cement is made by raw materials such as limestone, clay, etc., after a process of calcination. Raw cement clinkers are hard, large and roughly rounded particles on a scale of centimeters. Raw cement clinkers were ground with some amount of gypsum into small cement grains in the miller. Hence, shape of final cement grains are tended to angular shapes as illustrated by Fig. 2.5(a) on a scale of micrometers. Polyhedra seem more reasonable for simulation of cement based on this consideration.

2.5 Summary

Particles used in concrete either aggregate or cement or minerals have irregular shapes. The definition or simulation of shape, therefore, is complex. Experimental approaches to shape analysis in conventional studies are reviewed in this chapter. Compared with other methods, stereoscopic image analysis method (SIA) renders a compromise between accuracy and sophisticated equipments. An experimental study on a specimen of real gravel was conducted using image analysis. The results show a sieve size is not a good representation of particle size. Only median axis is close to the sieve size. Three axes are distributed in three different bands. The results of other shape parameters show that these specimens are equidimensional and close to the results found by Barksdale, R.D. and Itani (1994).

A simulation strategy based on different origins of arbitrary-shaped aggregate is proposed, which adopted some experimental conclusions. Surface texture simulation can also be considered by this method. A flexible simulation strategy proposed in this chapter is developed based on the image analysis approach. 2D simulation as well as 3D simulation can take the shape information directly from image analysis of a particle. For hydration simulation, a study was conducted pursuing the assessment of physically more realistic shapes as the commonly employed spherical one. This study encompassed polyhedra and ellipsoids. Experiments by X-ray micro-tomography on real cement were used as reference. It was shown that a limited variation of octahedrons or flat ellipsoids can be considered optimum solutions. They offer
more realistic S/V-relationships as spheres, which is crucial for cement hydration (Bullard and Garboczi, 2006).
CHAPTER 3

NUMERICAL SIMULATION OF PARTICLE PACKING

Numerical simulation is an effective approach to studying particle packing problems. In this chapter, a Monte Carlo (MC) based random sequential addition (RSA) packing system is developed. The limitations and the possible improvements of this RSA system are also discussed. A discrete element method (DEM) packing system will also be introduced and applied in a comparison study. This DEM-based system is capable of realistically generating the granular structures like the ones encountered in concrete. The differences between RSA and DEM-based packing characteristics found in this study will reveal the advantages and limitations of each method.

3.1 Introduction

Particle packing is a phenomenon encountered in many fields and has therefore received wide attention by scientists and technologists. The particle packing phenomenon can be studied in different ways. Experimental research can provide general information that can outline the scope of the problem. Various particle types can be submitted to different packing methods to assess the influences of technical parameters involved. An example of a loose packing test is presented in Chapter 2. Of course, an experimental approach is limited by the required setup and by its laborious and time-consuming characters.

Numerical simulation methods could be developed due to advances in computer technology. A range of numerical packing systems have been developed using various algorithms. Generally, conventional packing systems can be divided into two groups (Williams and Philipse, 2003). Systems based on random sequential addition (RSA) employ a random generator algorithm to disperse particles in a mould. It is an approach purely relying on stochastic principles. Particles are sequentially generated on random positions. Overlap leads to rejection of the last generated particle. Such traditional systems generate more evenly distributed particle systems than met in practice, and neglect as a consequence phenomena such as flocculation, agglomeration and clustering. The particles are placed rather than packed. Therefore, it is impossible to achieve in an economic way packing densities relevant for concrete aggregate by such systems (Williams and Philipse, 2003; Stroeven et al., 2009b).

Concurrent algorithm-based simulation (CAS) systems have been developed, avoiding such limitations. They may still start from RSA procedures, although this is not a necessity. These systems can realistically simulate the particulate structure compared with traditional RSA system. Different strategies for incorporating particle interaction are followed, but in dynamic systems a so-called dynamic stage is doing this. As an important algorithm used by CAS systems, a discrete element method (DEM) is usually employed to simulate dynamic
interactions between particles. DEM was introduced by Cundall and Strack (1979) in rock mechanics. It can take into account the interaction forces between particles. Motions of particles are governed by the force interactions and current motion status. It has become a numerical method different from the continuum-based finite element method (FEM). Apart from DEM used in CAS systems, some other packing algorithms are also adopted. Williams and Philipspe (2003) used a mechanical contraction to densify the dilute particles system. Overlapping is avoided in an interactive manner (Williams and Philipspe, 2003). Other analytical-based algorithms are also used for densification and for avoiding overlap, such as particle readjusting used by Puatatsananon et al. (2008) and separation checks used by Hänner et al. (2006).

Table 3.1 shows some typical particle packing simulation systems. It indicates both RSA methods and CAS methods in vogue in different fields. CAS seems a method somewhat later developed but presently the leading direction. In this chapter, a Monte Carlo (MC) based RSA is introduced. Limitations and possible improvements of an RSA system will be discussed. The DEM-based CAS system, SPACE, will be introduced and used for comparison purposes.

Table 3.1 Some typical particle packing simulation systems

<table>
<thead>
<tr>
<th>References of models</th>
<th>Shape of particles</th>
<th>Classification</th>
<th>Application</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wittmann et al. (1984)</td>
<td>Circles, polygons, arbitrary 2D shapes</td>
<td>RSA</td>
<td>Concrete</td>
</tr>
<tr>
<td>Cooper (1988)</td>
<td>Spheres</td>
<td>RSA</td>
<td>Physics</td>
</tr>
<tr>
<td>Evans, et al. (1989)</td>
<td>Overlapping spheres</td>
<td>RSA</td>
<td>Fibers</td>
</tr>
<tr>
<td>van Breugel (1991): HYMOSTRUC3D</td>
<td>Spheres</td>
<td>RSA</td>
<td>Cement</td>
</tr>
<tr>
<td>Coelho et al. (1997)</td>
<td>Spheres, ellipsoids</td>
<td>RSA</td>
<td>Physics</td>
</tr>
<tr>
<td>Sherwood (1997)</td>
<td>Spheroids</td>
<td>RSA</td>
<td>Physics</td>
</tr>
<tr>
<td>Lin &amp; Ng (1997): ELLIPSE3D</td>
<td>Ellipsoids</td>
<td>CAS/DEM</td>
<td>Soil</td>
</tr>
<tr>
<td>Stroeven (1999): SPACE</td>
<td>Spheres</td>
<td>CAS/DEM</td>
<td>Concrete</td>
</tr>
<tr>
<td>Kochevets et al. (2000): ROCPACK</td>
<td>Spheres</td>
<td>CAS/DEM</td>
<td>Aerospace</td>
</tr>
<tr>
<td>Jia &amp; Williams (2001): DigPac</td>
<td>Pixel or voxel based shapes</td>
<td>CAS/DEM</td>
<td>Materials</td>
</tr>
<tr>
<td>Fu &amp; Dekelbab (2003)</td>
<td>Spheres</td>
<td>CAS/DEM</td>
<td>Concrete</td>
</tr>
<tr>
<td>Williams &amp; Philipspe (2003)</td>
<td>Spheres, spherocylinders</td>
<td>CAS</td>
<td>Physics</td>
</tr>
</tbody>
</table>

3.2 Monte Carlo based RSA method

The Monte Carlo (MC) method is a computer algorithm for calculating results based on repeating random sampling. It was widely used in physical and mathematical fields. Herein, it is used in the particle packing process as a RSA method. This study will highlight the characteristics of the RSA system.

The key factor of the RSA method is the random generator, which is governed by the computational algorithm and the initial seed. Pseudo-random number generators (PRNG) are frequently used for simulation (Luby, 1996). As a basic type of PRNG, the linear congruential generator is defined as:
Fig. 3.1 Particle size distribution (PSD) of (left) a 2D sample of circles and (right) a 3D sample of spheres

Fig. 3.2 (left) a square plane and (right) a cube used as the target container for circles and for spheres, respectively, a is the linear dimension of the square or the cube in simulation

\[ X_{n+1} = (aX_n + b) \mod m \]  

in which, \( a \) and \( b \) are constants, \( X_{n+1} \), \( X_n \) are recurrence numbers, and \( m \) is the maximum number that can be produced. In this study, a combination of linear congruential generators is used for a better representation of random number generation.

The developed system will be applied to simulate problems in 2D as well as in 3D. Groups of 40 circles in 2D space and of 40 spheres in 3D space are used as the basic samples in the tests. The particle size distributions (PSD) of the samples are plotted in Fig. 3.1. The circular and spherical particles will be generated in a target square or cube, respectively, by the RSA system (see Fig. 3.2). Each “particle” centre will be on a random location in the target space. Any overlap of “particles” or “particles” with wall of the container will lead to rejection and regeneration.

3.2.1 Size sequence and random number seeds

Size sequence of particle generation is of importance for a RSA system. Some tests show that size sequence of generation has direct influence on the calculation efficiency. For instance, in a 2D example with target density 0.48, particle generation can easily be realized with sequence from large to small, while this is almost impossible when starting with the
Fig. 3.3 Example of different particle structures based on initial different random seed numbers (target $V_r = 0.48$)

small particles. This is due to large particles requiring equally large free space during generation. Thus, initial larger available space gives higher possibility for fitting of such large particles. Therefore, generation of particles from large to small is the preferred option in RSA systems, so is adopted by conventional RSA systems.

On the other hand, the random seed number (as initial value in Eq. (3.1)) is the key factor controlling the distribution of particles, while generation algorithm and particle size distribution are fixed. A different number of random seeds will result in different packed structures, as 2D examples may demonstrate in Fig. 3.3. An average of around 2000 steps is enough for the generation, which is relatively fast by a normal PC. Therefore, different packed structures are easily achieved by specifying different random seed number. A representative study can therefore readily be performed by this system.

3.2.2 Influences of the target packing densities

As the target objective, packing density controls computational efficiency by the RSA system. A series of tests were conducted with different target packing densities, but with the same initial random seed number. The examples of visualized structures in 2D and in 3D are shown in Fig. 3.4 and Fig. 3.5. With given seeds, the maximum packing densities of particles in 2D and in 3D seem to be 0.632 and 0.342, respectively.

Higher packing densities are difficult to achieve, even with 1 million steps. The maximum packing density is higher in 2D packing compared with packing in 3D. The correlations of total generation steps (trial steps) with packing density in 2D and in 3D are plotted in Fig. 3.6. With an increase in target packing density, the number of trials steps is also increasing. When target packing densities in 2D and in 3D are set to above 0.6, the necessary trials steps
are increased dramatically. Packing particles in 2D is more efficient compared to packing in 3D.

With different random seed numbers, different structures can be produced as shown in the previous section. It is also possible to get a higher packing density when starting by other seeds. Fig. 3.7 shows the structures with higher packing density both in 2D and in 3D.

Fig. 3.6 Required number of trials steps for achieving target packing density in a series of RSA 2D and 3D packing simulations starting with the same initial random seed number

Fig. 3.7 Visualized (left) 2D and (right) 3D structures with higher packing density using different seeds as in Fig. 3.4 and Fig. 3.5
Chapter 3

3.2.3 Refinement of generation space

Initially, in the generation process of particles the full-size space of a square in 2D or a cube in 3D is used. The random location of a centre point will lead to situations where part of a particle will penetrate the rigid boundary. This violation of the boundary condition should be avoided, so the centre point is rejected and re-generation is necessary. Detection of overlap with the boundary requires a special algorithm and leads to extra work. Using a dynamic container, which considers the size of the trial particle, can increase packing efficiency.

Fig. 3.8 and Fig. 3.9 compare the normal and refined approaches in 2D and 3D, respectively. Obviously, the generation efficiency is dramatically improved by this refinement. The number of steps to arrive at the same packing density is significantly reduced by this measure in 2D. In the 3D simulation, the ultimate packing density is even increased, whereby the maximum number of steps is fixed at the level of 1 million.

3.2.4 Influence of boundary conditions

Models with rigid boundary conditions are conventionally used in the materials field to simulate the structure with wall effects. On the contrary, models with periodic boundaries
are used to simulate bulk material structure. So far, the developed Monte Carlo-based RSA model made use of rigid boundary conditions. Therefore in what follows, this approach will be expanded with the same algorithm to also encompass periodic boundary.

Fig. 3.10 shows for the 2D case, using the same particles as well as the same procedure, the data on packing density versus number of trials. Comparison allows drawing the conclusion that periodic boundaries are much more effective for particle packing with the RSA system, as convincingly revealed by Fig. 3.11. At the same packing density, models with periodic boundaries need fewer simulation steps compared to models with rigid boundaries. The model with periodic boundaries only needs 2250 steps to arrive at a packing density of 0.632, whereas this requires almost 30000 steps for the model with rigid boundaries. Additionally, particles can be packed more densely under periodic boundary conditions. A target packing density of 0.684 could also be realized under periodic boundary conditions; this is almost impossible in a model with rigid boundaries. This is also a reason that models with periodic boundary conditions are frequently used in RSA systems (Ye, 2003). Of course,

Fig. 3.10 2D example of particle structures generated in a container with periodic boundaries having different target packing densities due to an increasing number of steps, but based on the same initial random seed number. Note that grey parts of particles occur “periodic” (i.e., are included at the opposite side of the container); black parts of particles are effectively included in the target container.

Fig. 3.11 Comparison for the 2D case of trial steps versus packing density in successive containers with rigid boundary conditions and with periodic ones.
Fig. 3.12 Visually displayed particle structures simulated by the RSA system with periodic boundary conditions and packed to different target volume fractions

Fig. 3.13 Comparison as to number of trial steps and maximum density of packing in containers with rigid and periodic boundary conditions

limitations are inherently associated with the use of RSA systems, irrespective of the use of periodic or rigid boundaries. This will be discussed in Section 3.3.

A similar study was conducted in 3D. Fig. 3.12 presents an example of visually displayed models with periodic boundaries packed to different densities. Models with periodic boundaries are superior in packing efficiency, completely analogous to the 2D case (see Fig. 3.13). The packing density capacity is also highest in models with periodic boundaries (i.e., 0.56 compared to 0.45). When the sample would represent cement particles in the scale of micrometers, a w/c of 0.3 could readily be achieved by this RSA system with periodic boundary conditions (so, representing bulk properties only).

3.3 SPACE approach to particle packing

SPACE (Software Package for the Assessment of Compositional Evolution) is a CAS system based on a DEM algorithm. SPACE offers a dynamic solution for the particle overlapping problem by a Newtonian motion model (Stroeven, 1999). Initially, particles with predefined size distribution are randomly generated in a large container; a similar approach as followed in the RSA method. Impulse-contact-based interaction between particles will then apply to
Each particle. Location and orientation of each particle change during a time step based on Newton's law of motion. Gravity and friction can be applied to particles during packing. A restitution variable can describe the energy dissipation, which can control the agglomeration phenomenon. Size of the container is gradually reduced to densify the particle structure. The interactions will be stopped when certain conditions are satisfied, such as arriving at the required volume fraction. Fully compacted particle structures can be achieved by this process as described by Fig. 3.14. Even, the so called crystallization state can be simulated (Stroeven, 1999).

3.3.1 A comparison with an experimental approach to particle packing

For comparison and verification purposes, a simulation study has been performed for experimental structural investigations on concretes, in which 16 mm mono-sized ceramic spheres replaced the largest aggregate grain fraction (Stroeven, 1973). This allows for verification possibilities as to the realistic character of SPACE-generated particle packing with respect to composition as well as to configuration-sensitive parameters of material structure. This is targeted in this section. Due to size invariance of the simulation system, this will hold for aggregate and cement grain packing alike.

Concrete mixtures were designed with the Dutch standard N480. Basically, a fine aggregate (called gravel in what follows) of which all grains passed through the 11.2 mm sieve was mixed with different amounts of 16 mm mono-sized spherical ceramic (steatite) aggregate. The resulting sieve curves are presented in Fig. 3.15, and fall roughly inside the area indicated in the German building code of those days for proper mixtures. The three mixtures are based on 10%, 30% and 50% by weight of steatite in the total aggregate (a), respectively. Ratios of gravel to cement (g/c=4.4) and water to cement (w/c=0.5) were similar for all mixtures. So, w/c ratio, and w and c contents were different (Stroeven, 1973).

Three 250 mm concrete cubes were prepared per mixture, in addition to series of other specimens for a variety of different tests. Boundary layers with a thickness of about 1.5 times the maximum grain size were removed from all sides to yield 200 mm cubes for the investigations. One of the 200 mm cubes per mixture was serially sectioned into tiles with a thickness of about 11 mm, so that 34-38 section images were obtained per cube. Firstly, all section images were subjected to stereological approaches for quantitative image analysis,
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Fig. 3.15 Aggregate grading of three experimentally investigated mixtures

exclusively focusing on the amount and the distribution of the steatite grains. This provided information on composition as well as on 2D configuration of the particle sections. Secondly, the spatial position of all steatite spheres was reconstructed from measurements of three perimeter points per grain section and information on the respective positions of the section images in the cube. This allowed for a 3D assessment of the highly configuration-sensitive nearest neighbour distance distribution in the cube.

Two-phase systems were generated by SPACE, consisting of mono-sized 16 mm spheres and a uniform matrix. For that purpose, the appropriate volume fractions of aggregate were calculated from the weight proportions mentioned. This resulted in 9.2%, 22.6% and 36.9% by volume of aggregate per mixture. Next, the particle numbers per cube were calculated and subsequently dispersed in the dilute state in containers significantly exceeding the size of the cube used in the experiments. Thereupon, they were slowly compacted with the dynamic concurrent algorithm in SPACE to the 200 mm cube size and the proper compositions, shown in Fig. 3.16. It should be reminded that the major difference with the experiments was that a uniform matrix replaced the sandy mortar.

The most obvious way of comparing experimental mixtures (realcrete) and computational concrete (compucrete) is by way of the visual impression section images make. The successive section patterns vary of course in the experimental as well as in the simulation setting.
Nevertheless, in both cases we see particle clustering (i.e., locally forming groups of particles) and the patchy structure (Diamond, 2006), reflected in the 2D section images (Fig. 3.17); this is a natural particle packing phenomenon, indeed. The composition parameter areal fraction can be obtained properly also by RSA-based systems, of course. This would be trivial information in the present case, however, since in both settings the volume fraction of coarse aggregate is designed. The composition character is reflected by the Gaussian type of probability density function (pdf) for volume fraction in serial sections, as found in both settings.

The section images reveal fluctuations in the sizes of grain sections. Since this may be a somewhat configuration sensitive phenomenon, we will compare realcrete and compucrete on this aspect. The appropriate quantitative image information of seven randomly selected sections per cube is combined in the computer simulation approach. Because of labor-intensity, only single sections were used in the experimental approach. For a random dispersion of mono-sized spheres, the probability density function (pdf) of the section diameter, \( D \), will be given by:

\[
f(D) = D \frac{1}{D_o \sqrt{D_o^2 - D^2}}
\]

where, \( D_o \) stands for the diameter of the steatite spheres (Stroeven, 1973). This theoretical estimate of the pdf is obviously independent of volume fraction.

Figure 3.18 presents the pdfs (in the form of the discrete histograms) of the section diameters pertaining to the two extreme mixture simulations by SPACE, the estimates by Eq. (3.2), and the experimental data of the same mixtures. Differences between experimental data and theoretical prediction are minor. The small circles are easily overlooked in the

Fig. 3.17 Section images of realcrete (left) and compucrete (right) of two different volume fractions of coarse aggregate revealing particle clustering
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![Graphs](image)

**Fig. 3.18** Discrete pdfs of grain section sizes, $D$ (or grain section areas, $A$) of the two extreme mixtures, with $V_v = 9.2\%$, at the left, and $V_v = 36.9\%$, at the right

experiments, as becomes apparent by comparison. Theoretically, Eq. (3.2) reveals 13% of all circles to be smaller than half the grain size (of 16 mm). In the experiments, on average less than 10% was observed (Stroeven, 1973). The compucrete yielded average values based on 31 section images of 12.6% and 12.4% for the two extreme mixes. So, compucrete results are more close to theoretical expectations.

Final assessment of SPACE’s capabilities for producing realistic compucrete as to particle dispersion is on the 3D distribution of centre-to-centre distance of neighbouring particles ($\Delta_3$) in the 22.6% sample (see Fig.3.16), shown in Fig. 3.19.

In the experimental approach, the thickness of the serial slices was measured and the average thickness of the saw cut calculated. Next, three widely spaced points on each perimeter of all particle sections were manually recorded on real size images (i.e., coordinates were recorded on an underlying measuring tablet upon making a slight manual imprint). A reconstruction algorithm based on Pythagoras’ rule, the measured slice thickness, and the estimated average saw cut thickness, was used for derivation of sphere centre positions and radii. The small differences in Fig. 3.19 between information derived from realcrete and compucrete is primarily due to the relatively low sensitivity of the realcrete approach, yielding the small tail at the left, and the portion of spheres with a diameter

![Graph](image)

**Fig. 3.19** Frequency distribution in realcrete and compucrete of the nearest neighbour distance in space, $\Delta_3$, for the intermediate mixture with 16 mm mono size spherical aggregate
slightly less that the actual one of 16 mm in the experimental approach. Hence, the compcrete information is more realistic than that of the realcrete in this case.

The conclusion that can also be drawn is that a significant portion of the grains in realcrete and compcrete ends up in (near) contact situations. This holds for most of the grains in the mixture with \( V_v = 36.9\% \); an almost continuous grain skeleton has formed. This is reflected by the surface-to-surface nearest neighbour distribution (NND) of the compcrete presented in Fig. 3.20. Fig. 3.20 also reveals clustering tendency to increase dramatically at higher volume fraction. It should be reminded, however, that only the largest aggregate grain size fraction was considered. Hence, clustering tendency is far more pronounced when all sand grains would be considered too, as was accomplished by Chen on SPACE-produced compcrete (Chen et al., 2005). As stated earlier, this can hardly be investigated by RSA systems; practical and fundamental problems are in the way of finding economic and reliable solutions.

3.3.2 A comparison with RSA to particle packing

Packing simulations are also conducted in the DEM system with the same samples of particles in Section 3.2 for comparison purposes. Fig. 3.21 visually illustrates a particle
structure packed in nature's gravity field, and presents a plot of the local packing density distribution along the vertical \( y \)-axis. The final global packing density is around 0.73, which is influenced by the loose packing at the top and by the lower packing density near the walls. It is considerable exceeding the afore-discussed RSA packing trials. When the effects of the loose packed top layer would be eliminated, or when compaction had been used, packing density by DEM could have been even significantly higher. So, DEM method is more flexible and more realistic considering the real situation of materials structure (as a result of compaction by vibration or due to gravity, etc.).

### 3.4 Limitations and improvements of RSA system for mono-sized particle packing

#### 3.4.1 One crucial limitation of RSA system in the mono-sized packing

Validation of the SPACE approach to packing of mono-sized spherical ceramic aggregate has been accomplished by comparing with experimental data. This was described in section 3.3.1. The outcomes demonstrated that this sort of DEM-based packing system is suitable for simulating the packing of dense granular particle structures, even rendering the possibility of the reliable evaluation of structure-sensitive properties. An RSA method has been introduced for particle packing as a possible alternative in section 3.2. In this section we will continue to compare both approaches.

Packing of mono-sized ceramic spherical particles by the RSA system is a relatively easy task for relatively low target packing densities. But for a higher target density, calculation efficiency is low compared with packing with multi-size particles. Simulation of a packed particle structure is becoming more difficult when the target packing density is set to above 30\%. The mission with target packing density of 36.9\% is impossible with this RSA system. Visual display of models with particle packing densities of 9.2\%, 22.6\% and 30.1\% produced by the RSA system are given in Fig. 3.22. The comparisons of distribution of surface-to-surface NND with DEM system and RSA system can be seen in Fig. 3.23.

The average surface-to-surface NND in structures with volume fraction 9.2\% and 22.6\% by RSA and DEM system are 3.74, 1.26 versus 3.53, 1.22, respectively. It seems that surface-to-surface NND of structures by RSA system has a wider distribution versus a DEM system. In other words, particles generated by an RSA system have a more even distribution

---

**Fig. 3.22** Packed mono-sized particle structure with different packing densities produced by the RSA system
Fig. 3.23 Comparison of frequency distribution of surface-to-surface NND in structures by DEM and RSA systems; note that packing density of 36.9% could not be achieved by the RSA system, for which 30.1% is used as an attainable alternative density.

compared with a DEM system, which inevitably omit the phenomena of patchy nature (Stroeven et al., 2009b).

Figure 3.24 shows a possible cause for the low packing density by the RSA system in mono-sized particle packing.

As particles are randomly distributed in space without overlap, the initially placed neighbouring particles may have mutual space which is too small for the same size of particle that is placed at a later trial. Therefore, this space will be left as permanent pore in the mono-sized packing. But in multi-size particle packing trials by the RSA system, small pores (space) can easily be filled by smaller particles. Hence, packing by the RSA system is more effective for multi-size particles. Mono-sized particle packing can be seen as a prime limitation of the RSA system. On the contrary, particles tend to reach most suitable locations by mutual interactions in the DEM system. Hence, the main limitations by RSA system can be avoided by DEM packing, which we have demonstrated.

![Diagram showing the difference between trial and placed particles](image-url)

**Fig. 3.24** Limitations of RSA in mono-sized particle packing compared with multi-size particle packing (solid particles: initially placed; dashed particles are trial particle in space between solid particles)
3.4.2 An improved RSA system based on the limitation in the RSA system

Packing capacity of RSA systems is significantly restricted when dealing with mono-sized particles, as shown in section 3.4.1. Some efforts to improve RSA systems (William and Philipse, 2003; Puatatsananon et al., 2008) have been made for increasing the packing density capacity. Herein a more direct method will be used for improvement.

It was demonstrated in Fig. 3.24 that the nearest neighbour distance (NND) \( l \) is a crucial parameter governing success or failure during the placement (generation) process. \( l \) should be kept as small as possible to increase packing density. Only when the NND of the trial particle with other placed particles is below a certain value, the generation will be accepted. Of course, the other controllers, e.g. boundary effects and overlap prevention are still valid. This leads to a denser structure, of course at the expense of a larger number of trials. This method can be operated as partial controller or entire controller when generating the target particles. We will demonstrate its effect for simulating a 2D mono-sized particle packing.

1000 circular mono-sized (4 mm) 2D particles will be packed in a square container by the RSA system. Some models generated by the traditional RSA method are shown in Fig. 3.25, whereby density is increased to its maximum value of 0.530. This level of packing is close to results (0.547) found by Lubachevesky and Stillinger (1990) with a similar algorithm.

The packing of particles by the improved RSA system (RSA-2DI) using one NND as criterion can simply be illustrated in Fig. 3.26 (a) and (b), dealing with the first 5 and 100 trial particles, respectively. It shows the growth of a more appropriate and denser structure at each trial, because a newly generated particle is compulsory to find a place close enough to generated particles. By this improved generation algorithm, packing density of mono-sized particle can eventually be improved. Final packing density was increased to 0.574 by this system as shown in Fig. 3.26.

To achieve high random packing density, the geometric structure of packed particle should be more uniform. A lot of small pore spaces are left between links in Fig. 3.26, which can not easily be filled by mono-sized particles at a later stage of simulation. Hence, the generation algorithm can be further improved by adopting two NNDs as criteria for generation of particles. The trial particle is restricted to find a place close enough to two neighbour particles. Figs. 3.27 (a) and (b) give two illustrative impressions of generated structures with different numbers of particles by this new system (RSA-2DII).

![Fig. 3.25 Generated models with mono-sized circular particles by a traditional RSA system (packing density from low to high)_guarded]

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structures tend to be plane-filled, but still keep a random character. Of course, ordered structures can be manually generated to obtain a high packing density. However, ordered structures exist seldom in reality except in crystalline materials and are not pursued in this study. Therefore, the maximum packing density can be further improved by this NND system. An example of generated structure is shown in Fig. 3.27(c).

The random packing density of mono-sized particles can be improved at least to 0.623. This maximum packing density obtained by the improved RSA system is still low, when compared with the packing density (0.78) realized by the DEM approach in section 4.4. This can be conceived an inherent limitation of RSA systems for generation of mono-sized particles. Further criteria to get to higher density levels will dramatically increase computational time, so will not be discuss herein.

Similar algorithms can be applied for packing of 3D particles by the RSA system. As an example, packing of mono-sized ceramic particles will be used for this purpose. As shown in Fig. 3.22, the maximum packing density of 3D mono-sized ceramic spheres is only 0.301, which is still lower than what Cooper has found (0.383) (1988) based on the RSA system. He did not mention the boundary condition in his tests (Cooper, 1988), and as we have shown earlier (in Section 3.2), particles can be packed to a higher density when using periodic
boundaries. So, 0.30 might be the maximum packing density for 3D mono-sized particle in a rigid container. In analogy with the 2D RSA system, the possible number of NND criteria could be taken 3 in the case of the 3D system. The possible geometric structures generated with different numbers of NNDs as criteria are displayed in Fig. 3.28. If one NND has been set as the criterion, the packing structure will tend to a line linked shape. Some generated structures with different numbers of mono-sized particles are shown in Fig. 3.29. Line linked structures can easily be observed in packed structures. By this method, packed structures of 1376 mono-sized spherical particles can be plotted in Fig. 3.29. Finally packing density can further be improved to 0.343 by this system (RSA-3DI).

The line linked packed structures generated by the improved RSA system using one NND as criterion, shown in Fig. 3.29, enclose a lot of small spaces between the lines of particles. This left space cannot easily be filled by later trials of mono-sized particles. Therefore, two NNDs were used as criteria to generate a more acceptable structure and to increase packing density, as shown in Fig. 3.30. Compared with the structure in Fig. 3.29, this RSA-3DII system leads to a much more tight structure. However, the generated structure tends to a layered system with enclosed pores. This algorithm is also applied to the generation of 1376 mono-sized spherical particle to see its efficiency. Possible packing density by the

![Illustrations of possible structures using different numbers of NNDs as criteria: (left) one NND (RSA-3DI), (middle) two NNDs (RSA-3DII), (right) three NNDs (RSA-3DIII)](image)

![Generated structures with different particle numbers (a) 5 and (b) 100 and (c) with maximum density by an improved RSA system (RSA-3DI), using one NND as criterion](image)
RSA-3DII system was found improved to 0.369, as shown in Fig. 3.30(c).

The plane filled structure can further be improved by applying three NNDs as criteria. Possible particle structures generated by the improved RSA system (RSA-3DIII) are displayed in Fig. 3.28(c), whereby use was made of three NNDs as criteria. This structure is tending to a 3D space filled system. Two generated structures involving different numbers of particles are shown in Figs. 3.31(a) and (b). They compare favorably with the ones whereby a smaller number of NNDs was used as criterion (Fig. 3.29 and Fig. 3.30). The structure with maximum packing density generated by this improved system (RSA-3DIII) is plotted in Fig. 3.31(c). It shows that packing density can be improved at least to 0.404 by using three NNDs as criteria. Compared to the classical packing density (0.64) mentioned by Bernal and Mason (1960), packing density by this improved RSA system is still low. However, packing density by a DEM system can further reach to around 0.6 (He et al., 2008a). Therefore, random packing density by RSA system is still limited to relatively low levels. Only DEM can provide optimum solutions. But the relatively efficient generation by RSA at lower density level can be utilized as initial particle distribution in DEM approaches to spherical or arbitrary shaped particles, as we will show later.

![Fig. 3.30](image1.png)  
**Fig. 3.30** Generated structures with different particle numbers (a) 5 and (b) 100 and (c) with maximum density by an improved RSA system (RSA-3DII), using two NND as criteria

![Fig. 3.31](image2.png)  
**Fig. 3.31** Generated structures with different particle numbers (a) 5 and (b) 100 and (c) with maximum density by an improved RSA system (RSA-3DIII), using three NNDs as the criteria
3.5 How CAS packing of arbitrary shaped particles can benefit from RSA system

Advantage of RSA systems is their generation efficiency when dealing with relatively low particle packing density. Different distributions can easily be achieved using different random seed numbers. Therefore, it is a suitable approach to generating the initial state of particle distribution in DEM systems. As such, it has been introduced in the SPACE system, a concurrent algorithm-based DEM system for spherical particles (Stroeven 1999). Only the traditional RSA system is implemented in this system, which limits the initial packing density. Of course, SPACE uses a dynamic packing process to achieve a dense packed structure, which compensates for the initial limitation by RSA.

Compared with application of the RSA method in DEM packing of spherical particles, it is more complicated when dealing with non-spherical particles, especially with arbitrary shape. Some regular shaped particles, e.g. ellipsoid, spherocylinders, etc. (Williams and Philipse, 2003) can directly be generated by RSA systems, since overlapping detection can be theoretically expressed by mathematical functions. But direct generation of non-overlapping arbitrary shaped particles by an RSA system is relatively complicated. Here one simplified method will be used for this purpose.

An encapsulated model is designed to apply the RSA generation model in DEM packing simulation with arbitrary shaped particles. Any arbitrary shaped particle can be encapsulated in a circle (2D) or in a sphere (3D) with a radius from its mass centre to the most remote perimeter or surface node, respectively. In this way, generation of arbitrary shaped particles can easily be achieved by the RSA system without additional computational efforts. Hence, overlap of fictitious particles in the generated structure can be avoided meanwhile guaranteeing relatively high packing density (with maximum density of capsule spheres). With different initial random seeds and random distribution of the direction of the principal axes of the real particles, different random packing structures can be achieved with arbitrary shaped particles. This method can profitably be used to generate the initial stage of arbitrary shaped particles in the DEM packing system. Some illustrative material of 2D applications is shown in Fig. 3.32. With the help of the RSA system, different distributions

![Illustration of 2D encapsulated model for generation by RSA of arbitrary shaped particle system with different rotations of particles or different packing densities (number outside the brackets is density of the capsule disk; number inside the brackets is the density of inner particles)](image)

Fig. 3.32 Illustration of 2D encapsulated model for generation by RSA of arbitrary shaped particle system with different rotations of particles or different packing densities (number outside the brackets is density of the capsule disk; number inside the brackets is the density of inner particles)
and different (limited) packing densities of arbitrary shaped particle are readily obtained. Dense packed structures can later be achieved by employing DEM simulation in a second stage, whereby influence exerted by the initial geometric distribution can be emphasized. By this procedure, extreme computational demands can be reduced dramatically.

This encapsulated model can easily be extended to 3D generation of arbitrary shaped particles by an RSA system. Relative dense packing of encapsulated spheres can easily be generated by an RSA system. Random distribution of particle structure can be realized with arbitrary shaped particles randomly rotated in their corresponding capsule spheres. Two examples of generated structures with different packing densities are shown in Fig. 3.33.

Final packing density is relatively low in this example due to the low volume fraction of particle inside the capsule spheres. But it is still higher compared to a manual distribution for multi-size particles. Furthermore, different distributions can easily be achieved with different random seeds. As there is no limitation to the shape of the particles inside the capsule sphere and so on its generation, arbitrary shaped particles can easily be dispersed at relatively low density. For instance, any type of ellipsoid can be encapsulated in the spheres and generated by an RSA system. Some examples are presented in Fig. 3.34.

Of course, the encapsulated model is flexible of generating any type of arbitrary shaped particles. A last example is shown in Fig. 3.35, whereby 8000 particles are involved. Spheres (left) can contain either arbitrary shaped particles (centre) or ellipsoids (right): they are all equally distributed in 3D. The only limitation of the generation efficiency in this system is the RSA algorithm. Any improvement such as the ones discussed in section 3.4 can contribute to the efficiency and capabilities of the encapsulated sphere model.

---

**Fig. 3.33** Two 3D structures of particles with arbitrary shape with different packing densities generated by encapsulated model in a RSA system (number outside the blanket is density of the capsule sphere, number inside the blanket is the density of inner particles)
3.6 Summary

In this chapter, different algorithm-based approaches to particle packing simulation are reviewed. As the two major groups of packing systems, RSA-based packing system and DEM system are discussed and compared. The basic features of an RSA system are presented. RSA systems are more effective for multi-size particle packing at relatively low particle density. The limitation and possible improvements are also discussed and their impact demonstrated by examples. A DEM-based system, i.e., SPACE is used in a comparison study with experimental results and demonstrated to yield reliable data up into the high packing density range. Even, it can be used for the evaluation of structure-sensitive feature of material structure, which is impossible by RSA systems. A method also has been revealed for possible application of the RSA method in arbitrary shaped particle packing in a DEM system. At least, RSA is effective for distribution of particles at low densities that can form the initial stage in a CAS system. DEM approach to particle packing will be further elaborated and applied in packing of arbitrary shaped particles in Chapter 4.
NUMERICAL ASSESSMENT OF THE INFLUENCE OF SHAPE ON PARTICLE PACKING

Shape of particles plays an important role in their behaviour. Shape is also recognized as a major factor influencing particle packing in addition to particle size and packing method (German, 1989). Therefore, it should be carefully studied. Different numerical approaches can be used for studying particle packing, as introduced in Chapter 3. DEM offers advantages as compared with traditional RSA approaches in more realistically distributing particles (Stroeven et al., 2009b) as demonstrated in the previous chapter. Generally, the spherical shape is assumed in traditional approaches, although this is not a fundamental limitation of RSA. In Chapter 2 some shape simulation strategies were proposed for particles used in concrete, i.e., aggregate as well as cement grains. The most appropriate shape strategy is implemented in the DEM-based packing simulation system HADES, which is therefore used in this study. Focal point of study will, therefore, be the assessment of shape effects on packing. Some important basic characteristics will be discussed in this chapter on packing of arbitrary shaped particles, such as mass properties of particles, overlap and coordination number assessment in a simulated structure, etc.

4.1 DEM-based HADES approach to arbitrary-shaped particle packing

A new DEM system, i.e. HADES, is developed for making more realistic simulations by incorporating arbitrarily shaped grains. It is based on a contact mechanism that evaluates the interaction forces exerted between segmented surfaces of neighbouring particles. For that purpose, guard zones are defined around each particle (see Fig. 4.1).

Fig. 4.1 Example of interaction between two particles: T is the guard zone thickness of a particle. Surface tessellations and boundary forces in interaction zone are partly sketched.
When the distance between two segments is less than the extent of this guard zone, interactive forces between two segments will be activated. The contact forces are a function of distances and areas of segments. Several forces can be applied on a particle such as spring force, cohesion force, damping force and friction force, etc. (see Fig. 4.1).

Spring force represents a repulsive force between contacted bodies. For the case of Fig. 4.1, it can be expressed by:

\[
\overline{F}_{sl} = -\sum_{i=1}^{m} \sum_{j=1}^{n} f_{s} \cdot \overline{V}_{12j} \cdot (1 - \frac{d_{ij}}{T})
\]  

(4.1)

where, \( F_{sl} \) is the summation of spring forces on body 1; \( m \) is the number of nodes on body 1, which are within the boundary zone of body 2; \( n \) is the number of evaluation points on body 2, which are within boundary zone of body 1; \( f_{s} \) is the coefficient of spring force; \( \overline{V}_{12j} \) is the unit vector for point 1i to 2j; \( d_{ij} \) is the distance between 1i and 2j and \( T \) is the thickness of the guard boundary.

A cohesive force is applied to represent attraction between particles, which is expressed by:

\[
\overline{F}_{cl} = \sum_{i=1}^{m} \sum_{j=1}^{n} f_{c} \cdot \overline{V}_{12j}
\]  

(4.2)

in which the summation of cohesive forces on body 1 is \( \overline{F}_{cl} \) and \( f_{c} \) is a coefficient of cohesion.

A damping force can also be considered in the system. It is expressed by:

\[
\overline{F}_{dl} = -\sum_{i=1}^{m} \sum_{j=1}^{n} f_{d} \cdot (\overline{v}_{12j} \cdot \overline{n}_{12j}) \cdot \overline{n}_{12j}
\]  

(4.3)

where the summation of damping forces on body 1 is \( \overline{F}_{dl} \) and \( f_{d} \) is a coefficient of damping. Further, \( \overline{v}_{12j} \) is the relative velocity vector from point 1i to 2j and \( \overline{n}_{12j} \) is relative normal vector point 1i to 2j.

A friction force can be also considered in HADES. It is based on the dynamic friction equation and can be expressed by:

\[
\overline{F}_{f1} = -\sum_{i=1}^{m} \sum_{j=1}^{n} f_{f} \cdot F_{nor} \cdot (\overline{V}_{12j} \cdot (\overline{n}_{12j} / d_{ij})) \cdot \overline{n}_{12j}
\]  

(4.4)

where the summation of friction forces on body 1 is \( \overline{F}_{f1} \) and \( f_{f} \) is the coefficient of friction; \( F_{nor} \) is the value of a normal force on 1i due to 2j; \( \overline{n}_{12j} \) is the perpendicular vector of \( \overline{n}_{12j} \).

A 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 much like in FE approaches. The linear motion and rotational motion of a particle can be calculated by Newton’s law of motion. Linear motion can therefore be expressed by:

\[
\overline{a}_{1} = \frac{\overline{F}_{1}}{m_{1}} = \sum_{j=1}^{m} \frac{\overline{F}_{1j}}{m_{1}}
\]  

(4.5)
Fig 4.2 Illustrations of spring forces: (a) linear behaviour of spring (b) non-linear behaviour of spring between particles

where \( \ddot{a}_1 \) is the linear acceleration of body 1; \( \overrightarrow{F}_1 \) is the summation of forces acting on body 1; \( m_1 \) is the mass of body 1 and the summation of forces acting on node \( i \) is \( \overrightarrow{F}_i \).

Rotational motion is in accordance with Newton’s second law of motion expressed by:

\[
\ddot{a}_1 = \frac{\tau}{I_1} = \sum_{i=1}^{m} \ddot{d}_{0i} \times \overrightarrow{F}_i
\]  

in which \( \ddot{a}_1 \) is the angular acceleration of body 1; \( I_1 \) is the principal moment of inertia; \( \tau \) is the torque on body 1; \( \overrightarrow{F}_i \) is the tangential force on \( i \); and \( \ddot{d}_{0i} \) is displacement vector (a vector from the point from centre of mass to the point \( 1i \) where force is applied).

As the spring force is the main factor resulting from overlap or penetration of particles, the coefficient of spring force \( f_s \) in Eq. (4.1) can be further refined from linear to nonlinear, as illustrated in Fig. 4.2. In this case, \( f_s \) will be specified in terms of a low value \( f_s \) inside a range \( T1<T \). When particles come very close, corresponding to a small distance range \( T2 \) (\( T1+T2=T \) and \( T2<<T1 \)), \( f_s \) will be replaced by a (higher) value \( f_s' \). It is expected that \( T1 \) will be occupied in dense packing and \( T2 \) will be a reference for growth model, which will be discussed later.

4.2 Assessment of mass properties

Newton’s law of motion is underlying the dynamic stage in HADES. This involves linear and rotational motion according to Eq. (4.5) and Eq. (4.6), respectively. After the shape has been determined as discussed in Chapter 2, the mass properties of each particle, e.g. mass, the centre of mass, the moment of inertia, etc., should be assessed before trajectories of moving particles can be calculated. Uniform density inside an arbitrary shaped particle is assumed for simplicity reasons. Based on classical physics, the aforementioned mass properties can be assessed by means of Eqs. 4.7-4.9. Mass properties of a 2D shape can be calculated by replacing volume elements \( V \) by area elements \( A \) in these equations.

Successively, we compute the mass according to:

\[
m = \int m dm = \int \rho dV = \rho \int V dV
\]  

(4.7)
in which, $m$ is mass, $\rho$ is mass density and $V$ is volume, respectively, of a particle. Furthermore, we have:

$$
\begin{align*}
    x_c &= \frac{\int x \, dm}{m} = \frac{\int x \, dV}{V} \\
    y_c &= \frac{\int y \, dm}{m} = \frac{\int y \, dV}{V} \\
    z_c &= \frac{\int z \, dm}{m} = \frac{\int z \, dV}{V}
\end{align*}
$$

(4.8)

in which, $x_c, y_c, z_c$ are the coordinates of the centre of mass. The moments of inertia are defined as follows:

$$
\begin{align*}
    I_{ij} &= I_{ji} = \int_{m} ij \, dm = \rho \int_{V} ij \, dV, \quad \text{in case of} \quad i \neq j \\
    I_{ii} &= \int_{m} (j^2 + k^2) \, dm = \rho \int_{V} r^2 \, dV
\end{align*}
$$

(4.9)

in which, $i, j, k \in [x, y, z]$ and $r$ is the distance from $dV$ to axis $i$, as illustrated in Fig. 4.3.

For solving these integral equations, a triangle and a tetrahedron are used as basic building blocks for arbitrarily-shaped 2D or 3D bodies. Any particle can be subdivided into a number of triangles in 2D and tetrahedra in 3D space. Therefore, a calculation of mass properties of arbitrary shaped particles is converted to a calculation scheme of calculating these parameters for a large number of triangles or tetrahedra, as shown in Fig. 4.4.

![Fig. 4.3 Illustration for calculation of the moment of inertia of an arbitrary shaped grain](image1.png)

![Fig. 4.4. (left) Triangle elements and (right) tetrahedral elements of an arbitrary shaped particle in 2D and in 3D, respectively](image2.png)
Hence, mass properties of any arbitrary triangle can be expressed by:

\[
\text{Mass of a triangle: } \rho S_{ABC} = \rho \begin{vmatrix} x_A & x_B & x_C \\ y_A & y_B & y_C \\ 1 & 1 & 1 \end{vmatrix}
\]

(4.10)

in which A, B and C are shown in Fig. 4.4(left) and \( \rho \) is the surface mass density. The centre of mass of this triangle is:

\[
x_o = \frac{x_A + x_B + x_C}{3}
\]

\[
y_o = \frac{y_A + y_B + y_C}{3}
\]

(4.11)

For a random point R inside the triangle ABC, its position can be expressed by area coordinates

\[
x_R = x_A L_1 + x_B L_2 + x_C L_3
\]

\[
y_R = y_A L_1 + y_B L_2 + y_C L_3
\]

(4.12)

in which, \( L_1 = \frac{S_1}{S_{ABC}} \), \( L_2 = \frac{S_2}{S_{ABC}} \), \( L_3 = \frac{S_3}{S_{ABC}} \); \( L_1 + L_2 + L_3 = 1.0 \); and \( S_1 = S_{RBC}, S_3 = S_{RAB}, S_2 = S_{RCA} \).

Calculation of the mass and mass centre of an arbitrary tetrahedron (shown in Fig. 4.5) is accomplished by Eqs. (4.13, 4.14):

\[
m_{ABCD} = \rho V_{ABCD} = \rho \begin{vmatrix} x_A & y_A & z_A & 1 \\ x_B & y_B & z_B & 1 \\ x_C & y_C & z_C & 1 \\ x_D & y_D & z_D & 1 \end{vmatrix}
\]

(4.13)

in which, \( m_{ABCD} \) is the mass and \( V_{ABCD} \) is the volume of a tetrahedron, respectively. Moreover,

\[
x_o = \frac{x_A + x_B + x_C + x_D}{4}
\]

\[
y_o = \frac{y_A + y_B + y_C + y_D}{4}
\]

\[
z_o = \frac{z_A + z_B + z_C + z_D}{4}
\]

(4.14)

Fig. 4.5 Calculation of mass properties of a tetrahedron example
in which, \( x_0, y_0, z_0 \) are the coordinates of the centre of mass in a tetrahedron.

Similar as in the 2D space, the volume coordinates expression will be used for any point inside the tetrahedron ABCD by Eq. (4.15):

\[
\begin{align*}
  x_R &= x_A L_4 + x_B L_2 + x_C L_3 + x_D L_4 \\
  y_R &= y_A L_1 + y_B L_2 + y_C L_3 + y_D L_4 \\
  z_R &= z_A L_1 + z_B L_2 + z_C L_3 + z_D L_4
\end{align*}
\]

(4.15)

in which, \( L_1 = V_1/V_{ABCD}, L_2 = V_2/V_{ABCD}, L_3 = V_3/V_{ABCD}, L_4 = V_4/V_{ABCD} \), \( L_1 + L_2 + L_3 + L_4 = 1 \), and \( V_1 = V_{BCD}, V_2 = V_{ACD}, V_3 = V_{ABD}, V_4 = V_{AB} \).

Finally, the moment of inertia of an arbitrary triangle or tetrahedron as well as of an arbitrary shaped particle can be determined by combining Eq. (4.12) or Eq. (4.15) and Eq. (4.9). But in a DEM system, the principal moment of inertia should also be determined and all nodes on the body should be adjusted to the principal Cartesian coordinate system. To do so, all moments of inertia of an arbitrary shaped particle \( (I_{xx}, I_{yy}, I_{zz}, I_{xy}, I_{xz}, I_{yz}) \) are calculated by the afore-described method and then the eigenvalues and eigenvectors of the matrix can be computed with Eq. (4.16):

\[
\begin{bmatrix}
  I_{xx} & -I_{xy} & -I_{xz} \\
  -I_{xy} & I_{yy} & -I_{yz} \\
  -I_{xz} & -I_{yz} & I_{zz}
\end{bmatrix}
\begin{bmatrix}
  x \\
  y \\
  z
\end{bmatrix}
= \lambda
\begin{bmatrix}
  x \\
  y \\
  z
\end{bmatrix}
\Rightarrow \lambda_i \bar{v}_i
\]

(4.16)

in which, \( \lambda_i \) is the eigenvalue and \( \bar{v}_i \) is the eigenvector.

The eigenvalues of this matrix are also the principal moments of inertia and the corresponding eigenvectors indicate the directions of principal axes. An example of the calculation of mass properties of an arbitrary-shaped 3D particle is presented in Table 4.1.

<table>
<thead>
<tr>
<th>Shape illustration</th>
<th>Volume and the principal moment of inertia</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image" alt="Shape Illustration" /></td>
<td>( V = 84.418 )</td>
</tr>
<tr>
<td></td>
<td>( I_{xx} = 2.84001 \rho V ) ( I_{yy} = 3.90995 \rho V )</td>
</tr>
<tr>
<td></td>
<td>( I_{zz} = 4.65785 \rho V )</td>
</tr>
</tbody>
</table>
4.3 Growth model and overlap assessment for dense packing state

4.3.1 Growth model for densification

As introduced in Section 4.1, the guard zone and its build-in spring re-action is instrumental in realizing dynamic particle interference without overlap. But it also results in small boundary gap zones in the dense packing, shown in Fig. 4.6(a). It will reduce the possible packing density, which will limit its applications in the evaluation of packing characteristics. One possible solution of this problem is to let particles grow to fill up the gaps, like Fig. 4.6(b). Therefore, a growth model is developed for this purpose. To maintain its initial particle shape, growing in normal direction to the surface of a particle is compulsory. Normal direction of a line or plane segment can be analytically derived. For instance, the normal vector of a plane can be expressed by Eq. (4.17) or Eq. (4.18):

\[
\vec{N} = \nabla f = \begin{bmatrix} a \\ b \\ c \end{bmatrix}
\]

(4.17)

in which, \( \vec{N} \) is the normal vector; \( \nabla f \) is the gradient; and \( a, b, c \) are coefficients of a plane expression \( f(x,y,z) = ax + by + cz + d = 0 \).

\[
\vec{N} = \vec{l}_1 \times \vec{l}_2
\]

(4.18)

in which, \( \vec{l}_1 \) and \( \vec{l}_2 \) are two crossed vectors in the plane.

The growth direction at each node on the surface or boundary of a particle is calculated from the normal vectors of related segments. The growth value of any node is related to the given global growth thickness and normal vectors of related segments. Fig. 4.7 shows a growth value calculation of a corner node in a 2D particle. Growth value \( x \) at the edge point is calculated by \( t/\cos \phi \) in this case. \( t \) is the given global growth thickness value and \( \phi \) is governed by the neighbour normal vectors \( \vec{C}_o \) and \( \vec{C}_1 \).

One example application of a growth model in a dilute 3D shaped particle system is shown in Fig. 4.8. It shows that the growth model is an effective way to densify the packed structure. The particle shape can be kept constant during growth. However, the suitable growth value \( t \) should be specified when using this model. An overestimated growth value will result in significant overlap in the structure. This will be discussed later.

![Fig. 4.6 (a) Possible boundary gap zone in dense packing; (b) application of growth model](image-url)
4.3.2 Assessment of local volume (surface area) distribution

Local volume assessment is of importance for the evaluation of packed structures. Defining wall effects, like characterization of the ITZ, requires the assessment of the local volume distribution. For particles with a simple shape that can be expressed mathematically, the approach would be relatively easy. But for a packed structure consisting of arbitrary shaped particles, local volume calculation constitutes a complex problem.

To solve the problem, the packed structure is sub-divided by a number of parallel sections like in Fig. 4.9(a), perpendicular to one axis, i.e. $x$, $y$ or $z$. When the
volume between neighbour sections can be determined, the complete distribution of $V_T$ of the particles can be assessed, as well.

First of all, the boundaries of particles in the section plane can be determined, shown in Fig. 4.9(b). Next, the area of each particle section in the section plane can be determined. Average area fraction of particle sections is according to first order stereological theory an unbiased estimator of volume fraction of an isotropic 3D structure, $\bar{A}_v = V_T$. Therefore, the local volume distribution along an axis can also be calculated. Precision of calculation only depends on the number of sections, but not on the mesh fineness of particles. An example of local volume distribution of a loose packed structure of cubes is shown in Fig. 4.10. 100 intervals or sections are considered enough for getting reliable information. The distribution of local volume can accordingly be assessed, like in the example of loose packed tetrahedra shown in Fig. 4.11. Wall effects and gravity influence are clearly revealed by Fig. 4.11.

![Fig. 4.10](image1.png)

Fig. 4.10 (a) Visualized structure and (b) volume fraction distribution of loose packing of cubes based on different evaluation intervals

![Fig. 4.11](image2.png)

Fig. 4.11 (a) Visualized structure and (b) volume fraction distribution of a loose packed structure of tetrahedra without growth along axis x, y, and z
4.3.3 Overlap assessment

The growth model discussed in Section 4.3.1 is an effective way to densify the packed structure. But one problem that remains is how to estimate a reasonable growth value for the particles. For instance, different growth values (from 0.1~0.4 mm) are applied to a packed structure of arbitrary octahedra (maximum size is about 5 mm), shown in Fig. 4.12. The volume distributions of grown particles are plotted in Fig. 4.13. The sections structure will reveal overlap in the model with a large growth value. Therefore, overlap assessment is crucial for determining a proper growth value.

Volume of the different components in the grown particle system will fulfill the following expressions:

\[ V_w = V_p + V_s \]  \hspace{1cm} (4.19)

in which \( V_p, V_s \) and \( V_w \) stand for volume of pores, solid and composite system, respectively.

\[ V_s = V_{pa} - V_{ov} \]  \hspace{1cm} (4.20)

whereby \( V_{pa} \) is the volume of particles including overlap and \( V_{ov} \) is the volume of overlap.

\[ V_w = V_p + V_{pa} - V_{ov} \]  \hspace{1cm} (4.21)

The Task is to identify \( V_{ov} \) in Eq. (4.21) and to set an upper level to it so that evaluation of

![Fig. 4.12 Visualized packed structures of arbitrary octahedrons with surface texture at different growth levels](image)

![Fig. 4.13 Volume distribution of packed structures in Fig. 4.12 with different levels of growth](image)
packing density is correctly executed. For this purpose, a stereological method based on the Cavalieri principle (Howard and Reed, 1998; Stroeven and Hu, 2006) is employed for identification of overlap.

Based on this method, a series of parallel and equidistant section planes are applied to an arbitrarily shaped object, shown in Fig. 4.14. Volume of solid particles ($\hat{V}$) including overlap can be predicted by Eq. (4.22) from particle section areas and the section plane spacing. As point sampling offers also a unbiased estimation of area, volume calculation of solid particles can be converted as a consequence to a point counting operation, as expressed by Eq. (4.22).

$$\hat{V} = (T \cdot A_1) + (T \cdot A_2) + \ldots + (T \cdot A_n) = T \cdot \sum_{i=1}^{n} A_i$$  \hspace{1cm} (4.22)

where $A_i$ is the cross-sectional area on $i$th slice, and $T$ is the spacing between the section planes. The volume can be rewritten according to:

$$\hat{V} = T \cdot a \sum_{i=1}^{n} P_i = T \cdot (\Delta x \cdot \Delta y) \sum_{i=1}^{n} P_i$$  \hspace{1cm} (4.23)

in which $a/p$ is the area associated with each evaluation point in the $i$th slice, $P_i$ is the number of points inside the particle displayed in the $i$th section. $\Delta x$ and $\Delta y$ are shown in Fig. 4.14.

The volume of the container $V_0$ can be expressed also by this method:

$$V_0 = T \cdot a \sum_{i=1}^{n} P_{i0} = T \cdot (\Delta x \cdot \Delta y) \sum_{i=1}^{n} P_{i0} = T \cdot (\Delta x \cdot \Delta y) \cdot P_0$$  \hspace{1cm} (4.24)

Herein, $P_0$ is the total number of evaluation points inside the container.

This method offers an unbiased estimation of the container’s volume. Therefore, the volume fraction of the solid structure ($V_{S\vee}$) in which particles may overlap can be expressed by Eq. (4.25). Volume of overlap can be further calculated according to Eq. (4.19) and Eq. (4.20).

$$V_{S\vee} = \frac{\hat{V}}{V_0} = \frac{T \cdot (\Delta x \cdot \Delta y) \sum_{i=1}^{n} P_i}{T \cdot (\Delta x \cdot \Delta y) \cdot P_0} = \sum_{i=1}^{n} \frac{P_i}{P_0}$$  \hspace{1cm} (4.25)

Fig. 4.14 Illustration of Cavalieri method (after Howard and Reed (1998))
$P_0$ is an unbiased estimation of the volume of the container, as stated earlier. But the precision of calculation depends on the calculation precision of each component. In other words, point sampling influences the reliability of the calculated volume fraction of each component. One way to improve the calculation precision is increasing the number of evaluation points inside the container, as indicated in Fig. 4.15. An example in Fig. 4.16 presents volume fractions pertaining to the model with growth value of 0.4 mm in Fig. 4.12 analyzed by different numbers of evaluation points. Obviously, the precision of the evaluation is increased by increasing the number (number in one direction) of sampling points. The evaluation is found stable when the linear number of sampling points exceeds 50.

However, an excessive number of evaluation points will cause the computation time to increase too much. Therefore, another method of increasing the evaluation precision can be emphasized, in which the number of evaluation points can be kept low. For instance, we keep the linear number of evaluation points as low as 10, but increase the trial number. Meanwhile, $x_0$, $y_0$, $z_0$ values are randomly arranged within 0 and 1.0*T, as shown in Fig. 4.15. An example of volume fraction distribution of different components in 100 trials with the same structure is shown in Fig. 4.17(a). It reveals the value to fluctuate around the reference value (adopted from Fig. 4.16). The average value of different components with different trial number is shown in Fig. 4.17(b).

The calculation precision can be ensured in both calculation methods. But to arrive at the same precision, the latter method is more economical, and is thus being selected for evaluation

![Fig. 4.15 Increasing number of evaluation points to refine the results](image1)

![Fig. 4.16 Volume fraction of respective components in a packed model of Fig. 4.12 with growth value of 0.4 mm, analyzed by different linear numbers of evaluation points](image2)
4.4 Influence of particle shape on 2D packing

The DEM-based HADES system renders the possibility of simulating the packing of 2D arbitrarily shaped objects. The ellipse is selected as a starting point. Loose packing of ellipses in the gravity field is achieved without shaking and used for evaluation of shape effects. To eliminate the influence of wall effects, periodic container boundaries were applied at the lateral sides. 1000 mono-sized particles were 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 an ellipse, respectively. 8 types of ellipses with different elongation value ranging from 1.0 to 0.3 were selected in the packing trials. Loose packed final structures are displayed in Fig. 4.19.
Some examples of local packing density distributions in vertical direction are plotted in Fig. 4.20. The influence of the container bottom boundary (wall effect) is clearly revealed by the figure. The interfacial region is around 0.1 times of effective height of the container. Local packing density fluctuates slightly around the bulk value in the centre part of packing structures. The looser structure at the top is obvious shown in Fig. 4.20. Therefore, bulk packing density was defined as average local packing density in the central region between 0.1 and 0.7 normalized distance from the bottom in the latter evaluation case.

Circularity is defined as perimeter ratio of ellipse and circle with the same area \((A)\). Circularity was also used as a relevant parameter in shape evaluation along with elongation. Analytically, the perimeter \((p)\) of an ellipse can be calculated from:

\[
p = \frac{\pi (a + b)}{2} \left(1 + \frac{1}{4} h + \frac{1}{64} h^2 + \frac{1}{256} h^3 + \ldots \right) \tag{4.26}
\]

where, \( h = \frac{(a - b)^2}{(a + b)^2} \). But the perimeter, as well as the area of a simulated ellipse, can vary due to the discrete mesh. Final circularity of an ellipse can be calculated by:
4 Numerical Assessment of the Influence of Shape on Particle Packing

Fig. 4.20 Distribution of local packing density of ellipses with different elongation values as function of the normalized distance to the bottom

\[
\text{Circularity} = \frac{P_{\text{eq.\ circle}}}{P_{\text{particle}}} = \frac{2\pi(A/\pi)^{1/2}}{P_{\text{particle}}} \tag{4.27}
\]

This allows displaying loose packing density as a function of elongation and circularity of the ellipses, as accomplished in Fig. 4.21. With a diminishing value of elongation or circularity, packing density of ellipse initially increases to finally show a decreasing trend. Loose packing density is found dramatically reduced when elongation below 0.6. Similar tendency is reflected by the loose packing density versus circularity in Fig. 4.21(b). But distinct from Fig. 4.21(a), the decline in loose packing density with decreasing of circularity is almost linear.

Next, another important parameter of packed particle structure is evaluated: coordination number. It represents the number of neighbouring particles forming contact with a given particle, averaged over all particles. Coordination number is supposedly correlated with porosity and with packing density (German, 1989). Proper accuracy in the evaluation requires a sufficient number of nodes, which are used as the calculation points. When we proportionally to the structure’s linear dimensions increase the number of evaluation nodes, accuracy will improve but at the expense of a dramatically increased computational effort.

Fig. 4.21 Relationship of loose packing density with (a) elongation and (b) circularity of ellipses
An example of an evaluation pertaining to the packed structure of ellipses with elongation value 0.4 is presented in Fig. 4.22 as a function of the quantity of evaluation nodes. At a small number of evaluation nodes, the coordination number of the packed structure will be under-estimated. When node numbers increase, coordination numbers also rise. Coordination numbers finally reach a stable level at and above a certain number of evaluation nodes indicated as 20 by Fig. 4.22. Therefore, this level can be employed in studies to yield coordination number of appreciable accuracy.

Frequency distributions of coordination numbers in packed structures of mono-sized ellipses are presented for various elongation values in Fig. 4.23. The mode values tend to shift to somewhat larger values of coordination number at decreasing elongation value. This tendency is reversed at elongation values exceeding 0.6, at least partly as a consequence of a dramatically reduced packing density with elongation. Average coordination numbers of differently packed structures are plotted as functions of elongation, circularity and loose packing density in Fig. 4.24, reflecting aforementioned tendencies. The relationship of average coordination number (ACN) with packing density was not very explicit. However,
ACN is roughly increased with increase of packing density. It seems circularity is a slightly better evaluation parameter for assessment of shape on particle packing.

As an effective method for enhancing packing density, compaction is introduced and its influence assessed by a simulation of packed ellipses. Because lateral boundaries were periodic, a rigid top boundary with a certain pressure was applied for augmenting packing density of initially loose packed structures. A loose packed structure of spheres was submitted to two different compaction states as a test. Local packing densities in the packed structure with and without compaction in vertical direction are plotted for comparison purposes in Fig. 4.25. The influence of compaction is obvious; compaction can effectively increase packing density throughout the packed structure. A higher compaction level will result in a relatively high packing density and higher coordination number. But too large compaction will also lead to penetration of particles. So, a relative modest compaction is selected for the very study. An interfacial region can also clearly be identified near the rigid top boundary through which the compaction is introduced in the packing system. Various loose packed systems of ellipses having different elongation were subjected to compaction. Some of the results are shown in Fig. 4.26. The dense packing densities due to compaction are higher than the comparable loose packing densities shown in Fig. 4.27. Presented findings of 2D tests are corresponding to observations on ellipsoids in 3D by Williams and Philips (2003).
Fig. 4.25 Comparison of (a) local packing density and (b) frequency distribution of coordination number of packed structure of spheres with and without different compaction states (compaction I is higher than compaction II).

Fig. 4.26 Examples of packed structures of ellipses with different elongation under compaction.

Fig. 4.27 Relationship of packing density with or without compaction versus (left) elongation and (right) circularity of ellipses.
4.5 Influence of particle shape on 3D packing

A similar procedure is followed in the case of the 3D packing of mono-sized standard polyhedra (with facet number 4 to 8) and the arbitrary shaped particles of Fig. 2.18(b). 864 particles with sieve size 10 mm were used for each simulation. Fig. 4.28 visually illustrates some loose packed structures with several typical shapes. As facet number and sphericity are the sensitive parameter for these shapes, loose packing density is presented in Fig. 4.29 as function of these parameters (without the information of shape in Fig. 2.18(b) in Fig. 4.29(a)).

Sphericity is defined as surface area ratio of equivalent sphere with particle (both having equal volume). Loose random packing density is generally increased with increasing facet number and sphericity as similarly found in case of random dense packing (German, 1989). Both cases of packing density have revealed particle shape as an extremely important factor in particle packing. It seems that polyhedra with larger sphericity can be packed to higher density.

Dense random packing simulations with compaction have also been performed based on the aforementioned particle generation strategy. 216 mono-sized particles ($d=10$ mm) have been used for each packing model. No gravity is involved. Fig. 4.30 visually illustrates some packing structures of differently shaped grains. As sphericity is a sensitive parameter in these ten shapes (nine faceted polyhedra plus sphere), the relationship of sphericity and maximum packing density is shown in Fig. 4.31. Dense random packing density of tetrahedrons and cubes complies with findings in (German, 1989).

![Image of packing structures](image_url)

**Fig. 4.28** Mono-sized random loose packing states of particles with some typical shapes

![Image of loose packing density](image_url)

**Fig. 4.29** Random loose packing density as function of (left) facet number and (right) sphericity of particles shown in Fig. 4.28
Coordination number is an important parameter for evaluating packing efficiency. Similar as in 2D space, a numerical method is established for calculation of coordination number of a packed system of arbitrary-shaped particles. Certain additional mesh and evaluation points are applied to surface of particles for the assessment purpose. Its precision is related to the fineness of the evaluation mesh. Selecting a coarse mesh speeds up the calculation, but leads to biased results (viz. brown line in Fig. 4.32). Therefore, a refined mesh is required for accurate evaluation.

Fig. 4.30 Mono-sized random packing with particles having typical shapes: (a) tetrahedron (b) hexahedron (c) octahedron and (d) sphere, respectively

Fig. 4.31 Dependency of maximum packing density on (a) facet number and (b) sphericity of 3D particles shown in Fig. 4.30

Fig. 4.32 Frequency distributions of coordination number in a tetrahedron packing for different degrees of fineness of the evaluation mesh (different numbers represent fineness of mesh, with larger values representing a coarser mesh)
mesh should be applied for the calculation of coordination number. Fig. 4.32 presents various frequency distributions of coordination number based on different meshes (in the model of loose packed tetrahedrons of Fig. 4.11(a), particle number is 864). It demonstrates that a sufficiently fine mesh is crucial for obtaining coordination numbers with proper accuracy.

This method has been applied for the evaluation of coordination numbers in the random dense packed structures of Fig. 4.30. The distributions of coordination number with different shapes are presented in Fig. 4.33. The relationship of average coordination number (ACN) with sphericity and packing density are also plotted in Fig. 4.34. From these figures, we can find that coordination numbers in polyhedral packing are also not only related to packing density, but also related to shape. For instance, average coordination number of ordered packing of cubes is only 6, while packing density can reach to 1.0.

![Fig. 4.33 Frequency distributions of coordination number of dense packed polyhedra of different types](image)

![Fig. 4.34 Dependency of average coordination number in densely packed polyhedra of different types on (a) sphericity and (b) packing density](image)
4.6 Summary

In this chapter, a DEM based CAS system, i.e. HADES, is employed for packing of arbitrary shaped particles. The fundamental packing algorithms of this approach are introduced. A physical approach is developed for assessment of mass properties of an arbitrary shaped particle, which is crucial for motion calculation in a DEM system. A growth model is also employed for densification of the packed structure. Possible overlap in a growing complex structure is also assessed based on a stereological approach. A proper growth value can be derived by this method.

Some simulation results of packed ellipses in 2D reveal shape parameters, such as elongation and circularity, to have significant influence on particle packing. Similar to the packing of ellipsoids in 3D, ellipses with relative small elongation have higher packing density than obtained for circles (and spheres in 3D). Packing density of ellipses with large elongation or low circularity is also lower than that of circles. circularity seems an even better parameter than elongation for describing the influence of shape on packing characteristics. Compaction is an effective way for densification of the loose packed particle structure.

Packing results with 3D polyhedra both in loose or dense states demonstrate that shape exerts a significant influence on packing density. Polyhedra with large sphericity tend to high packing densities except for some special shapes such as in the case of dense packed cubes. Evaluation of the average coordination number reveals influences exerted by packing density as well as by particle shape. Compaction leads to an increase in average coordination number.

In summary, influences of particle shape as well as packing method are investigated by the DEM based packing system and obtained results are reported and discussed. The influence of particle size on packing characteristics will be discussed in Chapter 5.
CHAPTER 5

MULTI-SIZED PARTICLE PACKINGS AND OPTIMUM MIXTURES

Optimum packing of aggregate is an important aspect of mixture design, since it may reduce porosity of the mixture. It may also reduce the usage of paste and is thus of economic relevance. In Chapter 4, for the case of mono-sized particle packing the influence of particle shape on particle packing was demonstrated. Next, this study will be extended to cover the influence of particle size. Several mathematic packing models have been developed in literature for optimization of mixture design. However in this study, numerical simulation will be used as the main tool for this purpose. A basic, simple theoretical model is used for approximate assessment of mixture optimization. Calculation and simulation will start from a bimodal mixture that is based on the mono-sized packing experiences. Tri-modal and multi-sized particle packing will then be discussed to find the optimum mixture. This study will demonstrate that computer simulation is a good alternative for mixture design and optimization.

5.1 Introduction

Practical mixture design should not only consider the engineering requirements and economic aspects, but also the demands from construction practice, such as rheology, pumpability, finishability, etc. (Shilstone and Shilstone, 1989). Mixture optimization is aiming to satisfy these requirements (Shilstone, 1990). Considering it from engineering and economic viewpoints, concrete with larger amount of aggregate and higher packed structure is cheaper, has lower porosity and shrinkage, and could have higher performance. Therefore, optimized aggregate mixture design plays an important role in concrete technology. Moreover, cement blending has become a popular way to generate high performance paste for HPC or UHPC. On this level, particle packing phenomena are also of paramount importance even when inert mineral admixtures are used (Goldman and Bentur, 1993). This also holds for concrete with finer fillers such as limestone powder (Ingram and Daugherty, 1992; Bonavetti et al., 2003), quartz flour (Lawrence et al., 2003; Rahhal and Talero, 2005) or other inert fillers (Bentz and Conway, 2001). Optimization of blended cement mixture also partly relies on proper mixture design, which is based on optimized particle packing (Bui et al., 2005).

A number of mathematic packing models are developed in the past century (Jones et al., 2002), such as by Furnas (1929), Aim & Goff (1967), Toufar et al. (1976), Dewar (1986) and de Larrard (1989; 1999). Jones et al. (2002) evaluated some of these analytical models on the
basis of experimental investigation involving different aggregate mixtures and cement blending. They found the models proposing similar sieve fractions; so, they were reliable in case of similar mean size of two neighbour groups. Reliability diminished however when mean size ratio drops below 0.4. Further research should be done on the more fundamental models both considering particle size and particle shape (Jones et al., 2002).

In this study, initially a relatively simply theoretical method is used to predict the maximum packing density and to reveal the influence of particle size. First, mixtures are bimodal; next, this concept is extended to ternary (tri-modal) and multi-sized particles. Numerical simulations aim at investigating effects of geometric and technological parameters. However, they are also used for verification purposes.

5.2 Theoretical packing situation

5.2.1 Bimodal particle packing

Two important parameters have to be assessed in bimodal particle packing:

- Size ratio of the two particles used in optimized packing process;
- Volume proportions of the two batches of bimodal particles.

The relevant information can be determined by experimental or numerical approaches, but can as well be approximated analytically. This starts from a packed structure of the larger mono-sized particles 1. The smaller sized particles 2 will be used as filler for the pores of the packed structure (see Fig. 5.1). In the optimum mixture, the largest pore is just filled by the filler particle. When this is the case, the initial packed structure can be expressed as follows:

\[ V_w = V_{p1} + V_{p1} \]  
\[ (5.1) \]

where \( V_w \) is the total volume of the system; \( V_{p1} \) and \( V_{p1} \) are the volume of particles 1 and of the pores, respectively, in the initial mono-sized packing structure.

If it is assumed that volume fraction (or packing density) is an invariable for packing of mono-sized particles 1, i.e. smaller sized particles 2 will only fill in the pore of initial mono-sized packed structure without disturbing the initial structure of particles 1. Therefore, it yields:

\[ V_{p1} = V_{p2} + V_{p2} \]  
\[ (5.2) \]

Fig. 5.1 Illustration of ordered packing of bimodal mixture of spherical particles

\[ \text{Particle 1} \]
\[ \text{Particle 2} \]
where \( V_{p2} \) and \( V_{p1} \) are, respectively, the volume of particles 2 and of the pores left by the combined system of both particle sizes, as shown in Fig. 5.1.

As a consequence, the following expression is obtained:

\[
V_w = V_{p1} + V_{p1} = V_{p2} + V_{p2}
\]

(5.3)

5.2.1.1 Size ratio of bimodal particles and maximum packing density

Final packing density should be highest in the optimized packing structure. As \( V_{p1} \) is well-known for mono-sized random packing structures, the main problem is to obtain the highest value for \( V_{p2} \) or the lowest for \( V_{p2} \).

For instance, random dense mono-sized sphere packing density is approximately 0.64 (Bernal and Mason, 1960). It is size invariant. Hence, the maximum packing density in bimodal packing would be 0.87.

In the described model, the small particles 2 fill the pores of the packed ordered structure of mono-sized particles 1. But in practice, where the shape of pores will be irregular, the actual packing structure will hardly reach the maximum one. Since smaller particle have a better capacity to fill in irregular-shaped pores, higher maximum packing density of the mixture can be achieved by using smaller sized particles 2.

5.2.1.2 Proportions in optimized bimodal packing

Another problem focuses on the proportion of two differently sized particle in the optimum packing structure. As above stated, the proportion can be expressed as:

\[
P = \frac{V_{p1}}{V_{p2}}
\]

(5.4)

\[
V_w = V_{p1} + V_{p1} = V_{p2} + V_{p2} = 1
\]

in a normalized system. When the packing density of mono-sized particles 1 is denoted by \( \psi_{p1} \), Eq. (5.4) will yield

\[
P = \frac{V_{p1}}{V_{p2}} = \frac{\psi_{p1}}{\psi_{p2} \cdot V_{p1}} = \frac{\psi_{p1}}{\psi_{p2} \cdot (1 - \psi_{p1})}
\]

(5.5)

where \( \psi_{p2} \) is the packing density of particles 2 filling the pores of particles 1.

In an ideal situation (without considering influences such as wall effect, particle crystallization, local loose effect, etc.), \( \psi_{p1} = \psi_{p2} \). Hence:

\[
P = \frac{\psi_{p1}}{\psi_{p2} \cdot (1 - \psi_{p1})} = \frac{1}{1 - \psi_{p1}}
\]

(5.6)

For the case of random dense spherical packing, \( \psi_{p1} = 0.64 \). Therefore, the optimum proportion of large particles to small particles is 2.778. In other words, the large particles should consume 73.5 % of the global volume, when the packing density of the global system reaches its highest value.

5.2.2 Ternary particle packing

Based on the above stated bimodal packing, adding small particles in the mono-sized particle structure is an efficient way to improve packing density. As afore-demonstrated, it is
Theoretically possible to roughly predict the optimized proportions and maximum packing density. This should be verified by numerical experiments, of course. Next, packing is extended to the tri-modal mixtures. As for the bimodal packing, the main focus is on the optimized proportioning of particles fractions and on estimating maximum packing density. The solution can be visualized by the theoretical set up of Fig. 5.2.

It is assumed again that packing starts from the dense ordered packed structure of the largest fraction of mono-sized particles. Next, the median sized particles will be added into the pores of the initial structure up to maximum packing density. Finally, the smallest particles will be added to fill the pores left in the bimodal packed structure. So, the complete system can be expressed by:

\[
V_w = V_{\text{pa1}} + V_{\text{p1}} = V_{\text{pa1}} + V_{\text{pa2}} + V_{\text{p2}} = V_{\text{pa1}} + V_{\text{pa2}} + V_{\text{pa3}} + V_{\text{p3}}
\]  

(5.7)

Of course, each fraction of particles can attain the maximum packing density of mono-sized particles in the ideal situation. Therefore, maximum packing density can easily be predicted by

\[
\psi_w = V_{\text{pa1}} + V_{\text{pa2}} + V_{\text{pa3}} = \psi_{\text{pa1}} + (1 - \psi_{\text{pa1}})\psi_{\text{pa2}} + [1 - \psi_{\text{pa1}} - (1 - \psi_{\text{pa1}})\psi_{\text{pa2}}]\psi_{\text{pa3}}
\]  

(5.8)

Hence, if density of randomly packed mono-sized spheres is 0.64, the maximum packing density of ternary sized spheres can attain 0.95. Similar as in the bimodal packing situation, smaller particles have a better flexibility to fill in the irregular pores between larger particles. So, this maximum packing density is only possible when there is a wider gap between neighbour particles.

Another goal is to obtain optimized proportions for each fraction of particles. For this purpose, \(P_1\) and \(P_2\) define the volume proportions of large to median particles, and of the large to small particles, respectively. This leads to:

\[
P_1 = \frac{V_{\text{pa1}}}{V_{\text{pa2}}} = \frac{\psi_{\text{pa1}}}{\psi_{\text{pa2}} \cdot V_{\text{p1}}} = \frac{\psi_{\text{pa1}}}{\psi_{\text{pa2}} \cdot (1 - \psi_{\text{pa1})}}
\]  

(5.9)

\[
P_2 = \frac{V_{\text{pa1}}}{V_{\text{pa3}}} = \frac{\psi_{\text{pa1}}}{\psi_{\text{pa3}} \cdot [1 - \psi_{\text{pa1}} - (1 - \psi_{\text{pa1})}\psi_{\text{pa2}}]} = \frac{\psi_{\text{pa1}}}{\psi_{\text{pa3}} \cdot (1 - \psi_{\text{pa1}} - \psi_{\text{pa2}} - \psi_{\text{pa1}}\psi_{\text{pa2})}}
\]  

(5.10)

**Fig. 5.2** An illustrative ordered tri-modal packed structure of spheres
In an ideal situation, the packing densities of the three particle fractions will be similar; so, $\Psi_{pa1} = \Psi_{pa2} = \Psi_{pa3}$. Hence, Eq. (5.9) and Eq. (5.10) simplify to:

$$P_1 = \frac{1}{1 - \Psi_{pa1}}$$

$$P_2 = \frac{1}{1 - 2\Psi_{pa1} - \Psi_{pa1}^2}$$

For the case of random dense packing of spheres, $\Psi_{pa1} = 0.64$. Optimized proportions of particles from large to small should therefore be 67.1%:24.2%:8.7%.

5.3 Computer simulation approach

5.3.1 RSA approach to bimodal particle packing

Particle packing is partly a geometric problem without considering the packing process. Any geometrically possible structure of discrete particles can render a packed structure. RSA computer simulation can be employed as a simple way to realize bimodal particle packing, avoiding the mixing problem. Although packing density by traditional RSA system is low compared with reality or with results by DEM simulation as shown in Chapter 3, properties of bimodal packing can still be addressed by this system.

Different bimodal circular (in 2D) and spherical (in 3D) particle packing situations with different size ratios were for this purpose approached by a traditional RSA system; the respective size ratios were 1:1.33, 1:2, 1:4, and 1:8. A total of more than 1000 particles are used in the simulation to fulfill the relevant RVE requirement (German, 1989).

The maximum packing density of mono-sized circular (2D) and spherical (3D) particles achieved by a traditional RSA system were shown to be about 0.524 ($\Psi_{pa1}$=0.53) and 0.31 ($\Psi_{pa1}$=0.3), respectively. Therefore, we can use the aforementioned theoretical set up to roughly predict the optimum proportions of bimodal mixtures and their maximum packing density. The large particles in 2D and in 3D should consume 68% and 59% by volume of the container, assuming $\Psi_{pa1}=\Psi_{pa2}$. Maximum packing densities are 0.78 and 0.51 for mixtures in 2D and in 3D based on Eq. (5.3), respectively.

The maximum packing density are found out by the RSA system in models with different volume ratios of bimodal particles (1:9, 3:7, 5:5, 6:4, 7:3, 9:1). Final example visualized packed structures in 2D and in 3D are shown in Fig. 5.3 and Fig. 5.5, respectively. Their corresponding bimodal particle packing results are presented in Fig. 5.4 and Fig. 5.6.
Fig. 5.3 2D examples of packing by a RSA system of bimodal particles with different size ratios (small: large): (a) 1:1.33; (b) 1:2; (c) 1:4; (d) 1:8; ratio in bracket is the volume ratio of large to small particles. Also the maximum packing density is given.

Fig. 5.4 Maximum packing density versus composition of bimodal mixtures for different 2D circular particle size ratios obtained by a RSA packing system (d1 and d2: sieve sizes of large and small particles, respectively)
Adding small particles to mono-sized packing of larger particles can generally improve packing density. Packing density of a mixture reaches a peak value where optimum mixture conditions are achieved. The peak of packing density is also influenced by the size ratio of particles involved. This holds both in 2D and 3D. When the size ratio of large to small particles is below 2 in 3D simulations, optimum is obtained for 70% large particles in the

Fig. 5.5 3D examples by a RSA system of bimodal particles with different size ratios (small: large): (a) 1:1.33; (b) 1:2; (c) 1:4; (d) 1:8; ratio in bracket is the volume ratio of large to small particles. Also the maximum packing density is given.
Chapter 5

0.3 0.35 0.4 0.45 0.5

0% 20% 40% 60% 80% 100%

Packing density (-)

$d_1/d_2=1.3$

$d_1/d_2=2.0$

$d_1/d_2=4.0$

$d_1/d_2=8.0$

$mixture. The optimum amount of large spherical particles declines to about 60% when the size ratio considerably exceeding the value of 2. Also, maximum packing density (peak value) is increased at higher size ratios. Obviously, smaller particles are more effective fillers when considerably smaller than the large particles. When compared to the theoretical prediction, we observe a better compliance for bimodal mixtures with larger particle size ratio.

Generalizing from the theoretical approach, we can see that maximum packing density is always obtained when the large particles occupy a major part of the total volume. Although small particles are more flexible in filling irregular pore size between large particles, increase in packing efficiency is slow when size is dramatically reduced. Moreover, segregation will become a problem under such conditions (de Larrard, 1999).

5.3.2 RSA approach to ternary particle packing

Similar as the above analysis, the RSA method is employed for ternary particle packing. Packing simulation will start from a 2D structure, whereupon a 3D structure will be approached. Basically, the maximum packing density of circles in 2D and spheres in 3D by a traditional RSA system are 0.524 and 0.310, respectively. Therefore, the maximum packing density and proportions of each phase in 2D or 3D can be approximated. The proportions of large particles to median and to small particles in 2D and in 3D are 58.73:27.96:13.31 and 46.17:31.85:21.98, respectively. Maximum packing densities in 2D and in 3D are 0.892 and 0.672, respectively.

A ternary dimension is used to clearly indicate the proportions of each phase of particles, shown in Fig. 5.7. Each corner of the equilateral triangle represents a mixture with hundred percent of a single particle fraction (large, median or small). Proportions of the three fractions of particles are indicated inside the triangle. Using the traditional RSA system, the maximum packing density can be assessed for each combination of particles, so the triangle can be completely covered by these data.
5.3.2.1 RSA approach to tri-modal packing in 2D

The RSA system is employed for calculating the maximum packing density of each combination of ternary particles. The size ratio of large particle to median particle and to small particle is set to 8:4:1. Fig. 5.8 visually displays at each node in the triangle the models at maximum packing density achieved by the RSA system. These values of a maximum packing density are presented in Fig. 5.9(a).

Next, in Fig. 5.9(b) the contour lines of maximum packing density are shown. The highest packing density is reached inside the red contour line, which includes the theoretical prediction of optimized proportions (58.73:27.96:13.31).
5.3.2.2 RSA approach to tri-modal packing in 3D

The size ratio of the three particle fractions are selected similar as in the former case of ternary 2D packing, i.e., 8:4:1. 3000 particles are considered in the simulation. Different combination of the three particle fractions are simulated by RSA to find maximum packing density. Results are visually displayed in Fig. 5.10. Quantitative values of maximum packing densities are shown in Fig. 5.11(a).
5 Multi-sized Particle Packing and Optimum Mixtures

Fig. 5.11 (a) Value distribution and (b) the corresponding contour lines of maximum packing density of ternary 3D particle mixtures

Fig. 5.11(b) presents the contour lines for maximum packing density, indicating inside the red contour line optimized proportion of ternary sized particles leading to highest densities, also including the theoretical solution (46.17:31.85:21.98).

5.3.3 DEM approach

Particle packing by a DEM system more realistically simulates the actual situation in practice. The same sequence of operations as accomplished by RSA will be followed.

The 2D bi-modal models are shown in Fig. 5.12 for different mixture proportion. The size ratio is 2. Loose packing and dense packing with compaction are both used for each mixture. Final packing densities are plotted in Fig. 5.13 for the various mixture proportions and each packing method. Besides the mono-sized particle packing, the packing density is initially enhanced with increased usage of large particles. A peak value was roughly obtained when the mixture contained about 70% of large particles (especially in models with compaction). The theoretical estimate amounts to 80%; further a maximum packing density of 0.94 is predicted.

Dense packing is largely influenced by so called crystallization (ordering), as can be seen in Fig. 5.12. Introducing a sufficient quantity of small particles will disturb this ordering in structure formations and thus will cause the packing density to decline, as demonstrated in
Fig. 5.12 Visual display of 2D models of bimodal particle obtained by a DEM system (size ratios 1:2): (a) loose packing; (b) dense packing due to compaction.

Fig. 5.13. It is expected that this phenomenon is less significant in 3D simulation. Crystallization will also be suppressed in DEM-generated irregularly-shaped particle packing, as demonstrated in Fig. 5.14 where ellipsoids with different aspect ratio have been simulated in the loose packing state; at higher elongation or aspect ratio, the “crystal” phenomenon is less significant and effects of filler are more obvious.

Fig. 5.13 Packing density in loose and compacted state of different bimodal mixtures obtained by a DEM.

Fig. 5.14 Bimodal packing in 3D of ellipsoids with different elongation or aspect ratio (size ratio =2).
5.4 Multimodal particle packing

Basically, adding smaller particles can increase the packing density of a whole system, which has been illustrated by bimodal packing and tri-modal packing. A theoretical framework for multimodal packing can be developed analogously as for bi-and tri-modal packing. So

\[ V_n = V_{pan} + V_{p1} + V_{p2} + \cdots V_{pn} \]

(5.13)

in which \( V_{pan} \) is the volume of nth particles and \( V_{pn} \) is the volume of pore left by nth particles. Each sized fraction can presumably arrive at a similar maximum density under “ideal” conditions. This renders the possibility of predicting total packing density of a whole system. The only variable is the packing density of mono-sized fraction of largest particles. The optimized proportions of each size fraction can also be roughly predicted by:

\[ P_n = \frac{V_{pan}}{V_{pan}} \cdot \left[ 1 - \frac{\psi_{pan}}{\psi_{p1}} \cdots \left( 1 - \frac{\psi_{pan}}{\psi_{p(n-1)}} \right) \right] \]

(5.14)

in which \( P_n \) is the volume ratio of the largest particles to that of the nth size fraction of particles. The adoption of the aforementioned “ideal” conditions leads to further simplification of Eq. (5.14). It can also be expected that optimum proportion ratio of two sized particles are maintained, which also has been illustrated by bimodal and ternary expectation.

Of course, the actual packing state will be influenced by many factors in reality, e.g. shape of particle, packing methods, physical interaction between particles, wall effects, etc. But basically, mono-sized packing should be treated as the most important one, from which multi-modal mixing can be developed. Influence of particle shape on packing is also revealed in mono-sized particle packing. When particle packing is only emphasized as a geometric problem, the influence of shape on multi-sized particle packing can be considered by incorporating information of mono-sized particle packing. For instance, eigen packing density of each constituent should be calibrated and used to calculate the combination of each size class in de Larrard’s models (LPM or CPM model) (de Larrard, 1999). Loose effects and wall effects are also analytically considered, which constitutes also the link to the rheology of concrete in those models (de Larrard, 1999).

One popular way of characterizing particle size fractions in concrete is Fuller’s curve developed by Fuller and Thomson (1907). This curve is given by:

\[ P(D) = \left( \frac{D}{D_{max}} \right)^q \]

(5.15)

in which \( P(D) \) is the cumulative volume percentage passing sieve size \( D \); \( D_{max} \) is the maximum grain size in the mixture; \( q \) is an exponent, originally specified as 0.5.

Different values of \( q \) ranging from 0.3 to 0.5 were later proposed by other researchers. It has been proven that \( q=0.45 \) leads to optimized mixtures for asphalt concrete (Roberts et al., 1996). Andreasen and Andreasen (1930) suggested \( q=0.37 \) for optimized packing. The curve with \( q=0.30 \) is close to the grading curve used by Su et al. (2001) for self-compacting concrete (SCC) (Brouwers and Radix, 2005). Curves with different values of \( q \) are plotted in Fig. 5.15 (a). It shows the curve to shift upwards for lower \( q \)-value; this implies that larger quantities of fine particles are involved. The finer particles are relatively scarce by the traditional Fuller
curve. Optimum grading in SCC should involve more fine particles compared with traditional Fuller-based concrete.

The Fuller curve describes the whole range of particle sizes downscaled to micro-level. But for practical use or for simulation, the curve can be restricted to a limited range of particle sizes upward from a minimum aggregate size (Brouwers and Radix, 2005)

\[ P(D) = \frac{D^q - D_{\text{min}}^q}{D_{\text{max}}^q - D_{\text{min}}^q} \]  

where, \( D_{\text{min}} \) is minimum particles size.

Some curves with different value of \( q \) and 1 mm for minimum particle size are presented in Fig. 5.15(b). Differences in the curves are smaller than in Fig. 5.15(a) for the standard Fuller curves. Next, simulations are conducted with the RSA method to check the influence of PSD governed by the modified Fuller curves on packing density. An example of visually displayed models and the packing density distributions are shown in Fig. 5.16. The influence

![Graph showing the Fuller and modified Fuller particle size distribution curves with different power numbers](image)

**Fig. 5.15** (a) Fuller and (b) modified Fuller particle size distribution curves with different power numbers

![Models and packing densities](image)

**Fig. 5.16** (a) Visually displayed models of RSA-packed particle structures (left column: \( q=0.5 \), right column: \( q=0.3 \)) and (b) packing densities for different values of \( q \) in modified Fuller curves
of $q$ is found insignificant. Decreasing the power number, packing density is slightly diminished at lower $q$ value due to larger amount of fines involved in the mixture, especially in models with periodic boundaries. The results still show that modified Fuller particle size distributions are optimum with $q$ 0.5 or 0.45.

5.5 Summary

Influences of particle size on particle packing are studied as the main objective in this chapter. A simple theoretical concept is employed for assessment of the influence of particle size on packing and for prediction of ideal optimum mixture. The numerical approach by the RSA system is then used for packing simulation. The analytical as well as the simulation approach go from bimodal packing to ternary packing. The results obtained by the RSA system comply well with the theoretical estimates. Although many other parameters are not taken into consideration such as particle shape, boundary conditions or interactions between particles, this analytical approach can still predict the mixture properties reasonable well. Introducing finer particles in mono-sized particle structures is an effective way to improve particle packing density. Simulations by the DEM approach in 2D space reveal that the effects of filler can be overtaken by the crystal phenomenon. In other words, particle interaction can be the dominant factor in achieving high packing density in some cases. Basically, an RSA system cannot reproduce this phenomenon. In packed systems of irregular shape particles this crystallization phenomenon is suppressed and the filler effect more significant. In multi-sized particle packing, optimum mixture can be calculated based on each mono-sized particle packing as in de Larrard’s models (de Larrard, 1999). The influence of particle shape can also be derived from mono-sized packing information. The simulation results show that packing density of particles based on modified Fuller curves reaches to a peak value when the power number $q$ is 0.5 or 0.45.
CHAPTER 6

INFLUENCE OF PARTICLE PACKING ON ELASTIC PROPERTIES OF CONCRETE

Concrete is a complex composite material. Hence, the main components of concrete on meso-scale should be considered when studying its global elastic properties. As a main ingredient of concrete, aggregate will exert influences on the elastic properties of concrete. In the present study, particularly particle shape and particle packing are considered of paramount importance. The densely packed structure of arbitrary shaped aggregate is simulated by the concurrent algorithm-based discrete element modelling (DEM) system HADES. A comparison is pursued of data, produced by numerical models, either based on arbitrary angular-shaped particles or on spherical ones. This will be accomplished by means of the finite element method (FEM). The results can be used to evaluate the adequacy for this purpose of conventional numerical or analytical models based on spherical aggregates. The influences exerted on the elastic properties of concrete by other factors, such as the mechanical and physical properties of the aggregate, the ITZ and the matrix will also be addressed in this study.

6.1 Introduction

Cementitious materials are of a particulate nature at different material scales. Aggregate while embedded in a cement paste is moulded to form the meso-structure of concrete during compaction by vibration. Cement particles are “compacted” during that process in water between the aggregate grains. This packing phenomenon is therefore relevant for concrete on meso-scale as well as on micro-scale. Packing of the major component of concrete, aggregate, occupying up to three quarters of its total volume, can directly affect the characteristics of concrete in the fresh state as well as in the hardened state. Dense random packing of aggregate is the normal situation in concrete. The particle packing simulation system should therefore have the capability of generating this dense random packing. This can be achieved by concurrent-algorithm-based discrete element modelling (DEM) systems.

The elastic properties of concrete play a crucial role in structural design and strength analysis (Pascale and Leo, 1979). Many studies have shown that meso-scale models are suitable for studying the global elastic properties of concrete. Extensive experimental studies have been conducted on the assessment of influences exerted by aggregate (Stock et al., 1979; Zhou, et al., 1995; Alexander and Milne, 1995; Sengul et al., 2002; Alonso et al., 2002), cement blending (Alexander and Milne, 1995; Nassif, 2005), curing conditions (Khaloo and Kim, 1999), test methods (Han and Kim, 2004), etc. (Wang et al., 1988; Oluokun et al., 1991; Piasta
and Schneider, 1992; Mangat and O’Flaherty, 2000; Sabeur et al., 2007; Dilek and Leming, 2008). The Young’s modulus and Poisson’s ratio are the two crucial elastic properties of concrete, so their prediction has practical significance. To approach this problem, analytical models (Nilsen et al., 1995; Yang, 1997; 1998; Geyskens et al., 1998; Zhao and Chen, 1998; Li et al., 1999; Garboczi and Berryman, 2001; Hashin and Monteiro, 2002; Nadeau, 2003; Demir, 2005; Zheng et al. 2006; Wang and Li, 2007; Sun et al., 2007) as well as numerical models (Li et al., 2003; Lilliu, 2007; Lee and Park, 2008) have been developed. For accurate prediction, all components of concrete should be taken into consideration, i.e., aggregate, matrix, ITZ, etc. (Nilsen et al., 1995). The main component, aggregate plays a major role, since its volume fraction can be as high as 0.70 or even 0.80. Previous studies have been focusing on size of the aggregate grains (Zheng et al., 2006; Li et al., 2003) as a major parameter. Spherically-shaped aggregate is normally considered in modelling approaches because of simplicity (Zhao and Chen, 1998; Li et al., 1999; Garboczi and Berryman, 2001; Li et al., 2003; Lilliu, 2007).

In this study, numerical meso-scale models are employed to assess the influence of particle packing on the elastic properties of concrete. However, contrary to the aforementioned studies, the influence of particle shape on packing properties will be additionally highlighted. A concurrent algorithm-based discrete element package can generate densely packed arbitrary-shaped aggregate grains in a cement matrix. When matured by hydration, this can be interpreted as a three-phase system.

Elastic properties of DEM-produced concrete, in which particle shape as well as packing density were varied, have been studied with the help of a finite element method (FEM). The results can be used to evaluate the adequacy for this purpose of conventional numerical or analytical models based on spherical aggregates in concrete. The influence of other factors on the elastic properties of concrete, such as the mechanical and physical properties of the aggregate, the ITZ and the matrix will also be discussed in this study.

6.2 Experiments

Since aggregate can take up as much as 80% of concrete’s volume, the concurrent algorithm-based simulation system HADES is employed to generate the packed meso-structure of concrete. This system allows arbitrary shaped particles to be compacted up to the dense random state. Only relatively coarse aggregate fractions are considered in this study for economic reasons. Since shape is a crucial factor to be emphasized in this study, both angularly-shaped as well as spherically-shaped grains will be employed.

A 3D packed aggregate structure consisting of irregularly-shaped octahedrons with imposed surface texture has been generated by HADES. Herewith, it is intended to simulate the crushed rock structure in compacted concrete (He et al., 2008b). Sections of the packed structure were selected for the numerical analysis. The initial packing density of 2~5 mm grains is around 0.4; see Fig. 6.1(a). Regarding the ITZ, a 3D growth model is employed with specific growth value to generate the ITZ region around the aggregate. The observed thickness of the ITZ around the various aggregate particles in the section planes will be different due to the geometric effect of the location of the section in the aggregate grains; observed 2D measures for ITZ extent will systematically exceed the real 3D thickness of the
Fig. 6.1 (a) Cube in which angularly-shaped aggregate grains are compacted by HADES system to desired density; arbitrary section through this 3D structure is indicated and displayed at the right (b), revealing the 2D pattern of the three phases involved. This sort of images is used in the 2D meso-scale model.

ITZ (Chen et al., 2003; Stroeven, 2000). This is a complicating phenomenon encountered in experimental evaluation of the ITZ’s width (Scrivener and Nemati, 1996).

A meso-scale model encompassing three phases is depicted by Fig. 6.1 (b). The models with circular aggregate are derived from those based on angularly-shaped grains, in a way discussed later.

After transferring geometric information from HADES to GMSH (Geuzaine and Remacle Webresource), the mesh will be applied to the selected sections. A meshed 2D example model is shown in Fig. 6.2 (a). The meshed model will then be transferred to the FEM system, so as to establish a numerical 2D concrete model. This preliminary study assumes linear

Fig. 6.2(a) A meshed model by GMSH and (b) established model in FEM subjected to the indicated boundary conditions
Computational Modelling of Particle Packing in Concrete: Chapter 6

elastic material behaviour. A group of basic material properties is assigned to the different phases, partly according to Li et al. (2003) following experimental results by Stock et al. (1979) as given in Table 6.1. The model is subjected to simple boundary conditions, as shown in Fig. 6.2 (b). Later, when the influences exerted by the different parameters are discussed, this basic material model will be used as a reference.

Table 6.1 Material properties of different phases applied in FEM

<table>
<thead>
<tr>
<th>Components</th>
<th>The Young’s modulus (GPa)</th>
<th>Poisson’s ratio (-)</th>
<th>Mass density (kg/m³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aggregate</td>
<td>75</td>
<td>0.15</td>
<td>2800</td>
</tr>
<tr>
<td>ITZ</td>
<td>7.2</td>
<td>0.35</td>
<td>1500</td>
</tr>
<tr>
<td>Matrix</td>
<td>12</td>
<td>0.25</td>
<td>2000</td>
</tr>
</tbody>
</table>

6.3 Theoretical background

6.3.1 Physical equations in theory of elasticity

In this study, two elastic parameters, i.e. the Young’s modulus and Poisson’s ratio, are analyzed. The theory of elasticity will be used for estimation purposes. Physical equations (Hooke’s Law in 3D) can be expressed for a Cartesian coordinate system by:

\[ \varepsilon_{11} = \frac{1}{E} \left[ \sigma_{11} - \mu (\sigma_{22} + \sigma_{33}) \right], \gamma_{23} = \frac{1}{G} \tau_{23} \]
\[ \varepsilon_{22} = \frac{1}{E} \left[ \sigma_{22} - \mu (\sigma_{11} + \sigma_{33}) \right], \gamma_{13} = \frac{1}{G} \tau_{13} \]
\[ \varepsilon_{33} = \frac{1}{E} \left[ \sigma_{33} - \mu (\sigma_{11} + \sigma_{22}) \right], \gamma_{12} = \frac{1}{G} \tau_{12} \]

where \( E \) is the Young’s modulus, \( \mu \) is Poisson’s ratio, and \( G \) defines the shear modulus. \( G = E/(1+\mu) \); \( \varepsilon_{11}, \varepsilon_{22} \) and \( \varepsilon_{33} \) are the strain components and \( \sigma_{11}, \sigma_{22} \) and \( \sigma_{33} \) the stress components in the direction of \( x, y \) and \( z \) axis, respectively. Further, \( \gamma_{23}, \gamma_{13} \) and \( \gamma_{12} \) are the angular strain components and \( \tau_{23}, \tau_{13} \) and \( \tau_{12} \) the shear stress components perpendicular to the respective orthogonal axes. This is illustrated in Fig. 6.3 (a).

Plain strain conditions are applied, so \( \varepsilon_{33} = \gamma_{13} = \gamma_{23} = 0 \). Hence, equation (6.1) yields:

\[ \varepsilon_{11} = \frac{1 - \mu^2}{E} \left[ \sigma_{11} - \frac{\mu}{1-\mu} \sigma_{22} \right] \]
\[ \varepsilon_{22} = \frac{1 - \mu^2}{E} \left[ \sigma_{22} - \frac{\mu}{1-\mu} \sigma_{11} \right] \]
\[ \gamma_{12} = \frac{2(1+\mu)}{E} \tau_{12} \]

Furthermore, the 2D model illustrated in Fig. 6.3 (b) will be employed. Vertical displacements will be applied to the top boundary. Horizontal boundary displacements are
allowed; only the bottom left point is fixed. Since no load is applied in horizontal direction, horizontal stress \( \sigma_{22} = 0 \). Therefore, equation (6.2) reduces to:

\[
\begin{align*}
\varepsilon_{11} &= \frac{1 - \mu^2}{E} \sigma_{11} \\
\varepsilon_{22} &= -\frac{\mu + \mu^2}{E} \sigma_{11} \\
\gamma_{12} &= \frac{2(1 + \mu)}{E} \tau_{12}
\end{align*}
\]  

(6.3)

Poisson’s ratio can be expressed in the model of Fig. 6.3(b) by

\[
\mu = \frac{1}{1 - \varepsilon_{11}/\varepsilon_{22}},
\]

with

\[
\frac{\varepsilon_{11}}{\varepsilon_{22}} = \frac{\Delta H}{H} = \frac{\Delta L}{L} = \frac{L \Delta H}{H \Delta L}.
\]

\( \Delta H \) and \( \Delta L \) are absolute values and all other symbols can be referred to Fig. 6.3. After substitution, this leads to:

\[
\mu = \frac{1}{1 - \varepsilon_{11}/\varepsilon_{22}} = \frac{H \Delta L}{H \Delta L + H \Delta H}
\]

(6.4)

Operating similarly, the Young’s modulus can be expressed by:

\[
E = \frac{1 - \mu^2}{\varepsilon_{11}} \sigma_{11} = \frac{1 - \mu^2}{\Delta H / H} \frac{F_R}{(L - \Delta L)T} = \frac{F_R \cdot H (L \Delta H + 2 L H \Delta L)}{(H \Delta L + L \Delta H)^2 (L - \Delta H)T}
\]

(6.5)

in which \( F_R \) is the applied load.

---

Fig. 6.3 (a) 3D stress components on infinitely small element; (b) sketch of 2D plane strain model used in this study
6.3.2 Upper and lower bound models for the Young’s modulus

For composite materials, Hashin-Strikman (H-S) (1963) developed the well-known stringent bounds for prediction of elastic moduli based on a two-phase model. However, this model is inadequate for the prediction of the elastic properties of concrete, due to its assumed three-phase nature (Nilsen and Monterio, 1993). Therefore, so-called series and parallel models can be used to roughly predict the elastic modulus of the three-phase composite material, as shown as Fig. 6.4. In case of unconstrained uniaxial tension (plane stress conditions), the Young’s modulus can be derived using these two models.

For series arrangement:

\[ E = \frac{\sigma}{\varepsilon} = \frac{F/A}{\Delta H/H} = \frac{FH}{A\Delta H} \]  
(6.6)

in which \(\Delta H = \Delta H_A + \Delta H_I + \Delta H_M = \frac{FH_A}{AE_A} + \frac{FH_I}{AE_I} + \frac{FH_M}{AE_M}\). Hence,

\[ E = \frac{HE_I E_M}{H_A E_I E_M + H_I E_M + H_M E_M} \]  
(6.7)

For parallel arrangement:

\[ E = \frac{\sigma}{\varepsilon} = \frac{F/A}{\varepsilon A} = \frac{F}{\varepsilon A} \]  
(6.8)

in which \(F = F_A + F_I + F_M = E_A \varepsilon A + E_I \varepsilon A + E_M \varepsilon A\). Hence,

\[ E = \frac{L_A E_A + L_I E_I + L_M E_M}{L} \]  
(6.9)

Fig. 6.4 Illustration of the two prediction models for the Young’s modulus: (left) series and (right) parallel arrangement of phases of the composite material.
Equation (6.7) and equation (6.9) constitute the approximate lower and upper bounds estimate for the Young's modulus, respectively. The models only incorporate volume fractions of the composing phases, *i.e.* aggregate, ITZ and cement paste in the present case. Since the elastic moduli are approximately structure-insensitive, this approximation will mostly be of practical value. The estimates by these two models will therefore be employed during this study. Nevertheless, the real material is more complicated; elastic moduli may be affected by other parameters, which is the topic of this study.

6.4 Parameter study

6.4.1 Influence of mesh fineness

Fineness of mesh is generally recognized as a possible influence factor in FEM evaluations. Particularly, it can be an important factor when dealing with arbitrary-shaped inclusions. Therefore, different fineness of mesh have been applied to the same composite model in which angularly-shaped aggregate particles at an area fraction of around 20% have been used, as depicted by Fig. 6.5.

The width of the ITZ is assumed to be 50 μm. The boundary conditions and loading process described in Fig. 6.3(b) were applied to these material models. The values of \( \Delta H \) and \( \Delta L \) are “measured” numerically. Values of elastic parameters (\( E \) and \( \mu \)) have been assessed using equations (6.4) and (6.5). The results show that between these models the maximum differences in elastic modulus and in Poisson’s ratio amount to 0.57% and 0.27%.

Fig. 6.5 2D meso-scale composite model is analyzed by applying different fineness of mesh ranging from relatively coarse in (a) to fine in (f).
respectively. The differences between the model in Fig. 6.5(c) and the model having the finest mesh (Fig. 6.5 (f)) is only 0.34% in the Young’s modulus and 0.21% in Poisson’s ratio. Hence, the mesh of Fig. 6.5(c) has been systematically used throughout this study. The mesh used in this study will not give rise to seriously biased results in the evaluation of elastic moduli.

6.4.2 Influence of aggregate
6.4.2.1 Influence of shape and packing of aggregate
Firstly the influence of shape as an important property of aggregate will be assessed in this study. 2D sections of the above-described 3D simulated angularly-shaped packed aggregate can be selected for application by FEM. The associated 2D model for spherical aggregate will be obtained by replacing angularly-shaped aggregate in sections by equivalent circles. An example is presented in Fig. 6.6. Each 2D angular aggregate has its corresponding circular aggregate keeping area fractions of aggregate and ITZ constant. Additionally, the location of mass centre of each aggregate section is similar in the two models. The width of the ITZ in the 3D model with angularly-shaped inclusions is 50 μm. Of course, the width of ITZ in 2D model with angularly-shaped aggregate varies at different locations due to sectioning process. These local variations in the 2D ITZ width are also copied in the model with circular aggregate sections. The material properties listed in Table 6.1 are assigned to each phase in the FEM approach. The boundary condition and loading process are the same for each model as described above.

Volume fraction (packing density) of aggregate is another important factor that will affect the elastic moduli. The different volume fractions (and thus, areal fractions) investigated for the two aggregate shapes are collected in Table 6.2. Particles are similarly dispersed at each volume fraction for the two different shapes. The results will reveal the influences of shape and of volume fraction of aggregate on the Young’s modulus. Predictions by series and parallel particle arrangement models will also be determined.

Data on the Young’s modulus for different shapes and volume fractions of aggregate are presented in Fig. 6.7 (left). Theoretical predictions are also given. The influence of shape of aggregate on the Young’s modulus of concrete is obviously only moderate. Angularly-shaped inclusions lead to higher Young’s modulus of concrete as in case of the

Fig. 6.6 Two meso-models of concrete containing differently shaped aggregate grains (left: arbitrary angular; right: circular), and applied mesh. Grain dispersion is similar in the two cases.
spherical aggregate, differences being at most only 3.6%. Volume fraction has a dramatic influence on the Young’s modulus. Experimental data are due to Stock et al. (1979). Stock et al. (1979) measured the modulus by the tension and compression tests. Fair agreement is found between numerical simulation results and the experimental data of reference Stock et al. (1979). Simulated Young’s modulus is indeed found situated between upper and lower bound predictions. The actual value of concrete is closer to the lower bound, i.e., as predicted by the series model. Deviations increase at higher volume fraction.

The second elastic property of the model concrete, Poisson’s ratio, is given in Fig. 6.7(right) for the two shapes at different volume fractions of aggregate. Poisson’s ratio decreases at higher volume fraction of aggregate, due to lower Poisson’s ratio of the aggregate. Shape of aggregate has modest influence on Poisson’s ratio of concrete; the angular aggregate leads to relatively lower values of Poisson’s ratio.

Fig. 6.7 (left) The Young’s modulus and (right) Poisson’s ratio of concrete composed of spherical and angular aggregate at different volume fractions. Experimental data are due to Stock et al. (1979).
Concrete containing the same amount of aggregate but with different shape will approximately have the same elastic parameters. Of course, properly compacted concrete can contain a higher volume percentage of spherical aggregate as compared to angularly-shaped aggregate (He et al., 2009a). So, concrete compacted into the state of dense random aggregate packing will have higher Young’s modulus and lower Poisson’s ratio when composed of the spherical type of aggregate. However, the stress distribution in the two concrete types is significantly different. This is reflected by Fig. 6.8. So, models containing aggregate with different shape can be expected having different fracture behaviour; this will be an important topic considered in Chapter 7.

For the further validation, an experimental study by Wang et al. (1988) can be used as a reference for evaluating data from the numerical approach with the same geometry data as Fig. 6.3(b). Wang et al. (1988) used an acoustic method to test the modulus in their experiments. The experimentally obtained values for the Young’s modulus of aggregate and matrix were 86.7 GPa and 30.13 GPa, respectively, and for Poisson’s ratios of 0.17 and 0.28, respectively. For the Young’s modulus and Poisson’s ratio of the ITZ, values of 24.1 GPa and 0.3 were taken from the literature (Li et al. 2003). The width of ITZ is assumed as 50 µm. The models with angular and spherical aggregate used in section 4.1 were employed in this evaluation. The results are shown in Fig. 6.9. The conclusion is that the numerical approach leads to reliable predictions for the elastic moduli. Trends revealed in Fig. 6.9 are similar as the ones discussed earlier.

So, evidence supports the conclusion that the shape of the aggregate has a minor influence on elastic parameters at equal amount of aggregate. Therefore, the numerical models (Li et al. 2003) or analytical models (Zhao and Chen, 1998; Li et al., 1999; Garboczi and Berryman, 2001; Li et al., 2003; Lilliu, 2007) based on the assumption of spherical shaped aggregate are suitable to predict the elastic parameters of concrete. Differences arise in practice, though, when both types of concrete are optimized with respect to maximum amount of aggregate. Under such conditions, density at the dense random packing state is higher for the spherical aggregate, so that the Young’s modulus will be higher and Poisson’s ratio will be lower than in the case of the angular aggregate.

Fig. 6.8 Maximum principal stress distribution in 2D model concretes subjected to the same uniform global tensile stress field with (left) angularly-shaped and (right) circularly-shaped aggregate grains at a volume fraction of 0.2
Fig. 6.9 (left) The Young’s modulus and (right) Poisson’s ratio of concrete composed of spherical and angular aggregate at different volume fractions. Experimental data are due to Wang et al. (1988).

Fig. 6.10 (left) The Young’s modulus and (right) Poisson’s ratio of concrete influenced by the elastic modular ratio of aggregate and matrix

6.4.2.2. Influence of stiffness properties of the aggregate

In practice, the stiffness of the aggregate can vary between wide limits. This holds for river gravel as well as for crushed rock. Lower values are obtained for light-weight aggregate. So, this is a factor to be considered in the numerical approach. A concrete containing (coarse) aggregate with a volume fraction of 0.466 is employed for this study as basic model. Elastic properties of the cement paste and of the ITZ are maintained as Table 6.1 in all models. Only the elastic properties of the aggregate will be varied (expressed by the ratio of elastic moduli of aggregate and matrix). The width of the ITZ is taken similar as before, i.e., $w_{\text{ITZ}} = 50 \, \mu m$.

Results are displayed in Fig. 6.10. The Young’s modulus of concrete is enhanced at higher elastic modular ratio of aggregate to matrix. This trend is non-linear; increases in the Young’s modulus of concrete are higher in the low-modular ratio range. The global value of Poisson’s ratio is also increasing at higher elastic modular ratio. The trend is similar as seen for the Young’s modulus.

6.4.3 Influence of ITZ

6.4.3.1 Influence of ITZ’s width.

The width of ITZ ($w$) is affected by properties of the cement paste, e.g., water to cement ratio,
mineral admixture, or cement type, etc. Estimated ITZ's thickness is also different (i.e., smaller) for structure-insensitive properties, such as approximately the elastic moduli, as for structure-sensitive ones, like crack initiation (Hu and Stroeven, 2004). The actual value of ITZ's width is of the order of tens of micrometers according to Zheng (2000). But hundreds of micrometers were frequently employed in numerical simulations because of limitations imposed by mesh or numerical approach (Lilliu, 2007). Hence, it is important to assess the influence of ITZ's width on elastic properties of concrete. For this purpose, a 2D model with angular aggregate at a volume fraction of 0.466 was selected as basic model. Different thicknesses of the ITZ were investigated in the initial stage, as shown in Fig. 6.11. The material properties of each phase are equal to the afore-mentioned ones. The same holds for the load-displacement conditions of the test. The final results are presented in Fig. 6.12.

It is clearly demonstrated by Fig. 6.12 that the elastic parameters are linearly dependent on the width of the ITZ. The Young's modulus increases, whereas Poisson's ratio declines at increasing width of the ITZ. This is due to ITZ's Young's modulus being lower and Poisson's ratio being higher compared with appropriate values of matrix or aggregate.

Fig. 6.11 2D meso-material models of angularly-shaped aggregate are shown at an area fraction of 0.446, whereby the ITZ width is gradually increased from (a) to (d).

Fig. 6.12 Influence of the width of the ITZ on (left) $E$ and on (right) Poisson’s ratio of concrete
6.4.3.2. Influence of elastic properties of the ITZ

Important for concrete are the mechanical properties of the ITZ, which are affected by properties of cement paste. The model is the same as indicated in section 4.3.1, whereby \( \text{w}_{\text{ITZ}} = 50 \, \mu m \) was chosen for evaluation purposes. Different mechanical properties, expressed by the elastic modulus ratio of matrix and ITZ, were applied to the model. The mechanical properties of ITZ and aggregate were kept constant. The boundary conditions and loading methods are all the same as in aforementioned models. The final results are shown in Fig. 6.13.

Figure 6.13(a) presents the relationship of the Young’s modulus of concrete versus elastic modulus ratio of ITZ and matrix. It demonstrates that improved properties of the ITZ can effectively increase the Young’s modulus of concrete. Conversely, this value will drop significantly when the elastic modulus ratio of ITZ and matrix will continue to decline below a value of 0.5. An opposite trend is observed for Poisson’s ratio of concrete in Fig. 6.13(b).

6.4.4 Influence of matrix (cement paste)

The properties of the hardened cement paste are affected in practice by the properties of the initial (fresh) mixture and the curing environment. Basically, different water cement ratios lead to differences in mechanical behaviour of the hardened cement paste. Of course, elastic moduli will also be affected. Furthermore, different water to cement ratios will also have impact on the properties of ITZ, e.g., the mechanical properties and width of ITZ. This has been discussed earlier.

To assess the influence of the matrix on the elastic moduli of concrete, the model used in section 6.4.3 with \( \text{w}_{\text{ITZ}} = 50 \, \mu m \) is employed. Changes in ITZ’s properties follow those in the matrix; the elastic modulus ratio of ITZ and matrix is maintained at 0.6. This primary study ignores the change in ITZ width due to variation in water to cement ratio of the matrix (Stroeven, 1999). The relationship of elastic properties of matured cement paste with water to cement ratio is adopted from data of Helmuth and Turk (1966) referenced by Sanahuja et al. (2007). In this reference, the Young’s modulus of cement paste is 13.8, 20.48, 28.8, 36.9 (GPa) with water to cement ratio in the fully hydrated state of 0.6, 0.5, 0.4, and 0.3, respectively. The properties of aggregate, and Poisson’s ratio of all material components are the same as those listed in Table 6.1. The final results are illustrated in Fig. 6.14.
The global value of the Young’s modulus of concrete declined significantly at higher water to cement ratio and decreasing the Young’s modulus of the matrix. Poisson’s ratio of concrete is increased at higher water to cement ratio. The influence of the water to cement ratio on the width of the ITZ has not been taken into consideration in this section. But the trend can be predicted. High water to cement ratio in the cement paste will result in somewhat increased width of ITZ (Stroeven and Stroeven, 1999; Hu and Stroeven 2004). Therefore, concrete with high water cement ratio will provide an additional contribution to the decline in the Young’s modulus of concrete based on the results of Fig. 6.12.

6.4.5 Influence of section locations
As the 2D models are selected from sections of 3D models, the location of sections is also expected to be a factor in elastic moduli evaluations. Therefore, a total number of 16 equidistant sections were selected to establish the 2D models. The material properties in Table 6.1 are applied to each model; ITZ’s width is 50 μm. The sections are listed in Table 6.3, whereby the x-coordinate indicates the location of the section in the 3D specimen.

Each section reflects a different area fraction of aggregate $A_A$ that is also listed in Table 6.3. The distribution of these area fraction data in the model material along the x-direction is shown in Fig. 6.15 (left). It complies with the global 3D packing density distribution along the x-axis as shown in Fig. 6.15 (right).
Table 6.3 Series of 2D sections selected from 3D model

<table>
<thead>
<tr>
<th>x</th>
<th>AA (%)</th>
<th>x</th>
<th>AA (%)</th>
<th>x</th>
<th>AA (%)</th>
<th>x</th>
<th>AA (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>-13</td>
<td>28.7</td>
<td>-12</td>
<td>42.6</td>
<td>-11</td>
<td>42.6</td>
<td>-9</td>
<td>43.3</td>
</tr>
<tr>
<td>-7</td>
<td>35.8</td>
<td>-5</td>
<td>39.1</td>
<td>-3</td>
<td>37.7</td>
<td>-1</td>
<td>39.8</td>
</tr>
<tr>
<td>+1.5</td>
<td>37.5</td>
<td>+3</td>
<td>43.2</td>
<td>+5.5</td>
<td>34.6</td>
<td>+7</td>
<td>32.0</td>
</tr>
<tr>
<td>+9</td>
<td>37.0</td>
<td>+11</td>
<td>49.3</td>
<td>+12</td>
<td>44.0</td>
<td>+13</td>
<td>25.4</td>
</tr>
</tbody>
</table>

Figure 6.16 (left) shows the distribution of the Young’s modulus along the normalized axis. The trend complies with the change of area fraction of aggregate in Fig. 6.15(left). Fig. 6.15 (left) Area fraction distribution of aggregate in sections and (right) packing density of 3D model along normalized x-axis
Fig. 6.16 (left) Distribution of the Young’s modulus along normalized x-axis, and (right) relationship between the Young’s modulus and area fraction of aggregate.

6.16(right) demonstrates that this is a direct consequence of the linear relationship of the Young’s modulus with area fraction of aggregate.

The Young’s modulus increases at increasing area fraction of aggregate. As a consequence, a totally reversed conclusion can be drawn for the correlation of the Young’s modulus of concrete with matrix area fraction as shown in Fig. 6.17(a). The relationship between the Young’s modulus and area fraction of ITZ is shown in Fig. 6.18(b). It demonstrates the relationship of the Young’s modulus of concrete and area fraction of the ITZ to be non-linear. The non-linear mutual dependence of area fractions of ITZ and aggregate, as revealed by Fig. 6.18(a) and (b), is due to the method of sectioning. Though the width of the ITZ in the 3D model is constant, particles are sectioned on variable distances to their centre, so that the 2D extent of the ITZ can fluctuate considerably. Hence, high area fractions of aggregate are not necessarily yielding high area fractions of ITZ. However, the area fraction of ITZ in this sample is relatively low compared to area fractions of aggregate and matrix. So, the aforementioned phenomenon does not resort in an observable effect on the relationship between the area fraction of aggregate (or matrix) and the Young’s modulus.

Poisson’s ratio is another important parameter investigated in this study. Fig. 6.19(a), (b) and (c) show the dependence of Poisson’s ratio on successive area fractions of aggregate,
Influence of Particle Packing on Elastic Properties of Concrete

Fig. 6.18(a) Relationship between area fractions of ITZ and of aggregate, and (b) distribution of area fraction of ITZ along x-axis

matrix and ITZ. Basically, Poisson's ratio increases at higher area fraction of matrix, whereas it declines at higher area fraction of aggregate. But the trend is also affected by the ITZ. So, Poisson’s ratio is affected by all three components, aggregate, matrix and ITZ. Compared with the observed tendency between the Young’s modulus and phase quantities, Poisson’s ratio of concrete is more sensitive to the ITZ phase. This yields in higher scatter around the trends in Fig. 6.19(a) or Fig. 6.19(b).

Fig. 6.19 Relationships of Poisson’s ratio with respective area fractions of (a) aggregate, of (b) matrix and of (c) ITZ
6.5 Summary

A meso-scale numerical model was used in this study to analyze the elastic properties of concrete. Both, angular-shaped and corresponding circular-shaped aggregate were used to assess influences on elastic properties. The Young's modulus increases at higher area fraction of aggregate and improved mechanical properties of aggregate, of matrix, and of ITZ. But the Young's modulus declines with increased extent of ITZ and at higher water to cement ratio. Poisson's ratio decreases at higher area fraction of aggregate and improved mechanical properties of ITZ, and of matrix. Contrary, it increases due to a larger extent of the ITZ, due to a higher water to cement ratio and at improved mechanical properties of the aggregate. Furthermore, Poisson's ratio was found more sensitive than the Young's modulus for effects exerted by the ITZ. The shape of the aggregate was observed having but marginal influence on the Young's modulus. So, the conclusion can be drawn that proper estimates on elastic properties of concrete can be derived from numerical and analytical models based on spherical grain shape, since grain shape only sorted minor influences. On the other hand, stress levels in models with differently shaped aggregate are different. So, fracture behaviour is expected to be different for concrete with different shape of aggregate. This will be pursued in chapter 7.
CHAPTER 7

INFLUENCE OF PARTICLE PACKING ON FRACTURE BEHAVIOUR OF CONCRETE

Particle packing on meso-level has a significant influence on workability of fresh concrete and also on the mechanical and durability properties of the matured material. In Chapter 6 it was demonstrated that shape exerted a marginal influence on the elastic properties of concrete particle compared to that of packing density. Hence, elastic properties of concrete can be treated as structure-insensitive parameters. However, fracture behaviour can be expected structure-sensitive. This is supported by the difference in stress level in model concretes containing aggregate with different shape as discussed in Section 6.4. Therefore, it is interesting and highly relevant to extend this study to assessing the influence of particle packing on fracture behaviour of concrete. Additionally, effects on fracture behaviour exerted by other parameters such as mechanical and geometric properties of the three phases will also be discussed here.

7.1 Introduction

Strength and fracture behaviour are regarded as major properties of concrete that are at the basis of structure design and analysis of this material. This field is extensively covered by experimental studies that mainly focus on influence caused by aggregate type (Tschegg and Elser, 1995; Akcaoglu et al., 2004; Yasar et al., 2004; Chen and Liu, 2004; Rocco and Elices, 2008; 2009; Tabsh and Abdelfatah, 2009), by w/c (Yasar et al., 2004; ), by loading types (Tschegg et al., 1995; Yan and Lin, 2006), by size effects (van Vliet and van Mier, 1999; Carpinteri et al., 2004), etc. (Stroeven, 1973; Almusallam et al., 2004).

Compared with the time-consuming experimental approach, numerical modelling constitutes a more flexible alternative. Numerical fracture models of concrete can be sub-divided into several groups such as continuum, discontinuous based on XFEM, discrete and lattice models (Lilliu, 2007). Continuum models conceive stress and strain as continuous throughout the material and include cracks smeared out over a region (crack band). As an example, a damage variable ω is employed in continuum damage models to specify deterioration of the stiffness matrix (Stroeven, 1973; Peerlings, 1999; Jirásek and Patzák, 2002). Non-local and gradient damage models are developed to reduce mesh sensitivity and damage localization (Brekelmans et al., 1995; Peerlings, 1999; Jirásek and Marfia, 2005; Ferrara and Di Prisco, 2001). Discontinuous models based on XFEM (Wells and Sluys, 2001) are used to model cracks that can arbitrary run through a mesh in a mesh-objectation manner. Discrete models treat materials as consisting of a numbers of rigid bodies. The
force-displacement bond is applied for neighboured particles (Vonk, 1992; Azevedo and Lemos, 2005; 2006). Lattice models separate the material into a number of beams or trusses (Herrmann, et al., 1989; Bažant et al., 1990; Leite et al., 2004). A purely linear elastic-brittle constitutive law can be applied to each beam in the lattice model (Schlangen and Garboczi, 1997; Lilliu, 2007).

Concrete is a heterogeneous material that can be treated as a three-phase composite on meso-scale. As the weakest part of normal concrete, the ITZ is regarded as the most feasible part for crack initiation and propagation. So, ITZs play an important role in fracture behaviour of concrete. On the other hand, aggregate takes up to three quarters of concrete’s volume. Hence, it also plays an important role in the mechanical properties of concrete. Shape is an important but complex property of the aggregate; so, conventionally, it is treated as spherical in numerical fracture analysis (Bažant et al., 1990; Azevedo and Lemos, 2005; Zhao and Hao, 2008). Concrete is a complex heterogeneous particulate material; yet, only limited literature is available dealing with the influences of particle packing on fracture behaviour of concrete (Du and Sun, 2007; Rocco and Elies, 2009).

This chapter will focus on the effect of shape of particles and particle packing on fracture behaviour of concrete. Meso-scale models will be established like in Chapter 6 and subjected to numerical fracture simulation approaches. Some basic conclusions will be drawn on the influences of shape and packing of aggregate on fracture behaviour of concrete. Some other effects exerted by mechanical and geometric properties of the three phases will also be discussed in this study.

7.2 Experiments

Generally, a similar procedure is followed for the generation of numerical models of the three-phase structure as in Chapter 6. A couple of meshed 2D example models with different shaped inclusions are shown in Fig. 7.1.

The meshed model will then be transferred to the FEM system, so as to establish a numerical 2D concrete model. Compared with the study of the elastic properties (Chapter 6),

![Fig. 7.1 Models with inclusions of different shape, (a) angular (b) circular, meshed by GMSH](image-url)
a finer mesh is necessary to achieve better fracture simulation results. A group of basic material properties is assigned to the different phases, partly according to Li et al. (2003) following experimental results by Stock et al. (1979) and Kwan et al. (1999b) as given in Table 7.1. The model is subjected to simple boundary conditions, as shown in Fig. 7.1. Later, when the influences exerted by the different parameters are discussed, this basic material model will be used as reference.

Table 7.1 Material properties of different phases applied in FEM

<table>
<thead>
<tr>
<th>Components</th>
<th>Young's modulus (GPa)</th>
<th>Poisson's ratio (-)</th>
<th>Tensile strength (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aggregate</td>
<td>75</td>
<td>0.15</td>
<td>40</td>
</tr>
<tr>
<td>ITZ</td>
<td>7.2</td>
<td>0.35</td>
<td>2.2</td>
</tr>
<tr>
<td>Matrix</td>
<td>12</td>
<td>0.25</td>
<td>6</td>
</tr>
</tbody>
</table>

7.3 Damage material constitution

In this study, a simple isotropic damage model (Jirásek and Marfia, 2005; Radtke et al., 2008) will be applied for the mechanical behaviour of each phase of concrete. The model describes the stress-strain behaviour of a material in which damage evolution takes place, such as expressed by Eq. (7.1) and Fig. 7.2.

$$\sigma = (1 - \omega) D \varepsilon$$  \hspace{1cm} (7.1)

in which $\sigma$ and $\varepsilon$ define stress and strain of the material, respectively; $D$ is the stiffness matrix of the undamaged material; $\omega$ is a damage scalar as defined by Eq. (7.2).

$$\omega = \begin{cases} 0 \\ 1 - \frac{\varepsilon_0}{k} \exp\left(\frac{k - \varepsilon_0}{\varepsilon_f - \varepsilon_0}\right) \end{cases}$$  \hspace{1cm} (7.2)

where $\varepsilon_0$ is the strain at peak stress, $\varepsilon_0 = f_t/E$, in which $f_t$ and $E$ are the tensile strength and elasticity modulus, respectively; $\varepsilon_f$ is a parameter specifying the slope of the softening branch; $k$ is a parameter related to the history of damage evolution.

![Stress-strain relationship in the damage model](image-url)
The damage energy release rate $Y$ is evaluated by means of the equivalent stain $\tilde{\varepsilon}$:

$$\tilde{\varepsilon} = \sqrt{\frac{2Y}{E}} = \sqrt{\frac{\varepsilon^T D \varepsilon}{E}}$$

(7.3)

To reduce the limitation of the isotropic damage model due to mesh sensitivity, energy regularization (Brekelmans et al., 1995; Radtke et al., 2008) is applied, with $\varepsilon_f$ defined by:

$$\varepsilon_f = \frac{\lambda}{h}(\varepsilon_f - \frac{\varepsilon_0}{2}) + \frac{\varepsilon_0}{2}$$

(7.3)

Herein, $\lambda$ is defined as the width of the damage zone and $h$ is a parameter related to the element size.

### 7.4 Parameter study

#### 7.4.1 Mesh sensitivity checked by a simple beam model

Mesh sensitivity is an inherent problem of traditional local damage models, so that reliability of numerical simulation largely depends on mesh fineness. As indicated before, an energy regularization method is applied for solving this problem. The efficiency of the resulting improvements is checked by a simple beam model shown in Fig. 7.3. The model is also composed of three phases, i.e. aggregate, ITZ and matrix, in a series arrangement. The material properties of the three phases comply with Table 7.1. Information on size, dimensions, loading and boundary conditions is given in Fig. 7.3. A slightly weaker section is designed in the middle of the ITZ region for localizing crack initiation and propagation. Different mesh finenesses are applied to this beam model, illustrated in Fig. 7.4. These three beam models are subjected to uniaxial tension.

The most important results of the tensile test are the force-displacement (F-D) curves presented in Fig. 7.5. The F-D curves of the three models are reasonably similar, despite the
relatively large differences in mesh fineness. The softening curves of the three models form a narrow band. Therefore, the adopted material damage model for fracture evaluation is considered suitable for this study. This simple beam model will also be used for evaluation of other parameters in the study, to be discussed later.

7.4.2 Influence of shape and packing density of aggregate
As prime objectives, the influences of shape and packing density of aggregate on fracture behaviour will first be evaluated. Meso-structure models with different volume fraction and shape of aggregate as shown in Table 6.2 were used in the uniaxial tensile test, similar as in the approach to the elastic properties. Material properties of each phase comply with Table 7.1. The width of the ITZ is also maintained at 50 μm. Resulting F-D curves of the various models are presented in Fig.7.6, where Aaa and Aac represent the area fraction of aggregate in the model with arbitrary angular particle shape and with circular shape, respectively.
The results in Fig. 7.6 demonstrate that models with circular-shaped aggregate have a relatively high tensile strength as compared to models with angular-shaped inclusions. This may be due to the high stress concentration in the case of the angular-shaped inclusions, which leads to an earlier crack initiation and development. Similar results were found by Du and Lin (2007) in a numerical comparison of model with polygonal and spherical aggregate. However, distributions of polygonal and spherical aggregate particle were different in comparable situations in their study; this may have exerted influence on fracture behaviour and is therefore considered in the present study. Fig. 7.7 shows the vertical displacement contours of models with the same aggregate volume density of 20.1%, however containing aggregate with different shape. Cracks are clearly delineated by the boundary between different colors. The figures indicate that cracks were first initiated in the relatively weak ITZs. Next, cracks propagate into the matrix to coalesce, forming the major crack in the model. The major cracks are roughly perpendicular to the loading direction and very similar in two models.

Another important objective pursued here is the influence of packing density of aggregate on fracture behaviour of concrete. Fig. 7.6 reveals tensile strength of concrete being reduced at increasing packing density of angular and circular aggregate grains. This is probably resulting from increased numbers of ITZ regions at higher packing density of aggregate. This promotes propagation and coalescence of cracks. Similar results on compression strength were found by Tasdemir and Karihaloo (2001). The results on ultimate tensile force for different models are presented in Fig. 7.8, revealing the changing effect of particle shape at increasing packing density.

It should be mentioned here that the tendencies revealed by the experiments largely depend on the properties of the ITZ. Fracture characteristics will change when the ITZ properties are modified with respect to those of the other phases. As an example, the mechanical properties of the ITZ in the meso-structure models are taken similar to those of

Fig. 7.7 Vertical displacement contour in model with (a) angular aggregate and (b) spherical aggregate (red to blue: large displacement to small displacement; line between red and blue delineates the major crack)
7 Influence of Particle Packing on Fracture Behaviour of Concrete

![Graph](image)

**Fig. 7.8** Ultimate tensile load in models containing aggregate with different shape at different volume fractions

![Graph](image)

**Fig. 7.9** F-D curves of models composed of cement matrix and aggregate with different shape at different volume fractions (no ITZ)

the matrix. In other words, the ITZ is omitted. The F-D curves for this case are given in Fig. 7.9, evidencing the significant impact of the ITZ on fracture behaviour of concrete. The shape of the aggregate has a smaller influence on fracture behaviour when the ITZ is omitted. The peak tensile force or tensile strength is slightly increased with increasing packing density of the aggregate. Hence, an opposite conclusion can be drawn in models without and with ITZ.

**7.4.3 Influence of mechanical properties of aggregate**

Firstly, the mechanical properties of the aggregate will be emphasized. Later, the influences exerted by other parameters such as the mechanical and geometric properties of the various phases will be evaluated. For that purpose, a basic model containing 42.7% by volume of arbitrary-shaped aggregate is selected, as shown in Fig. 7.10. Different mechanical properties are applied to the same meso-structure model. Thereupon, these models are subjected to the
tensile test. The material properties of ITZ are listed in Table 7.2.

The F-D curves pertaining to the models with different mechanical properties of aggregate are shown in Fig. 7.11. The results indicate that the mechanical properties of the aggregate have only minor influence on the fracture behaviour of concrete as long as the aggregate is stronger than the matrix. This is because aggregate grains are rarely cracked when stronger than the matrix. But when the mechanical properties are equivalent or inferior with respect to those of the matrix, the tensile strength drops dramatically.

### Table 7.2 Mechanical properties of aggregate used for comparison purposes in models

<table>
<thead>
<tr>
<th>Ratio of Young’s moduli of aggregate and matrix (E\text{agg}/E\text{matrix})</th>
<th>E of aggregate (E\text{agg}) (Mpa)</th>
<th>Tensile strength of aggregate (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.25</td>
<td>75</td>
<td>40</td>
</tr>
<tr>
<td>5</td>
<td>60</td>
<td>32</td>
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<td>3</td>
<td>36</td>
<td>19</td>
</tr>
<tr>
<td>1</td>
<td>12</td>
<td>6</td>
</tr>
</tbody>
</table>

Fig. 7.11 F-D curves of models with different mechanical properties of aggregate
7.4.4 Influence of width of ITZ

The influence on fracture behaviour exerted by the ITZ should be carefully studied. A crucial feature of the ITZ is its width; a parameter still discussed in the literature. Width of the ITZ depends on the sensitivity of the descriptor of material structure to particle configuration (Freudenthal, 1950; Hu and Stroeven, 2004), as demonstrated in a study on cement paste in Chapter 8. Zheng (2000) found analytically that the ITZ’s width will be in a range of tens of micrometers in concrete, supporting experimental evidence (Scrivener and Nemati, 1996). However, due to inherent difficulties in numerical simulations, the ITZ is frequently assumed hundreds of micrometers wide (Lilliu, 2007; Zhou and Hao, 2008). Thus, it is interesting and relevant to assess the influence of ITZ’s width on fracture behaviour of concrete. The basic model shown in Fig. 7.10 was used for this purpose, however imposing a variation in the width of the ITZ.

Hence, four different models with ITZ width ranging from 30 μm to 90 μm were generated, illustrated in Fig. 6.11. Next, these models were subjected to the tensile test. The obtained F-D curves and final vertical displacement contour of different models are presented in Fig. 7.12 and Fig.7.13, respectively.

Obviously, the width of the ITZ has a significant influence a fracture behaviour of concrete.

![F-D curves of models with similar aggregate structure, however with ITZs having different widths](image)

![Contour of vertical displacement at ultimate reveals crack paths at different width of ITZs](image)
Fig. 7.14 Beam models with different accumulated ITZ width (left to right: 1, 3 and 5 mm of ITZ, respectively)

Fig. 7.15 F-D curves of beam models of Fig. 7.14 with different ITZ width

Concrete, which is particularly apparent in the softening stage. Larger width of the ITZ gives rise to more ductile behaviour and slightly lower ultimate tensile strength. In other words, model with more extensive ITZ has enhanced energy dissipation capacity. This is due to the changes of the crack paths and so changes of the damage patterns and increased ITZ length, as illustrated in Fig. 7.13.

For more explicit demonstrating the influence of the ITZ width on composite behaviour, the simple beam model shown in Fig. 7.3 is used. Changing width of accumulated ITZ phase in beam model (1, 2, 3, 4, 5 and 10 mm, respectively) will generate models shown in Fig. 7.14. Next, these beam models are subjected to the tensile test. Resulting F-D curves are shown in Fig. 7.15. The curves indicate that a model with a larger ITZ with has a lower peak tensile force, which is similar but less apparent in Fig. 7.12. Softening behaviour is also similarly reflected. Therefore, the width of the ITZ should be considered an important parameter in fracture analysis of concrete.

7.4.5 Influence of mechanical properties of ITZ

Mechanical properties of the ITZ are directly related to the microstructure of the material. Different design parameters such as w/c, hydration duration, cement quality or cement blending will result in differences in material structure and thus is mechanical properties of the ITZ (Hu and Stroeven, 2004). Hence, different mechanical properties are assigned to the basic model in Fig. 7.10 to assess its effect on the fracture behaviour of concrete. The proposed material properties of the ITZ are assumed proportional to the properties of matrix; data are listed in Table 7.3.
Table 7.3 Different mechanical properties of ITZ employed in models for comparison purposes

<table>
<thead>
<tr>
<th>Ratio of Young’s moduli of ITZ and matrix ($E_{itz}/E_{matrix}$)</th>
<th>$E$ of ITZ (Eitz) (Mpa)</th>
<th>Tensile strength of ITZ (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.4</td>
<td>4.8</td>
<td>1.0</td>
</tr>
<tr>
<td>0.6</td>
<td>7.2</td>
<td>2.2</td>
</tr>
<tr>
<td>0.8</td>
<td>9.6</td>
<td>4.1</td>
</tr>
<tr>
<td>1.0</td>
<td>12.0</td>
<td>6.0</td>
</tr>
</tbody>
</table>

Achieved models are then subjected to a tensile test. Corresponding F-D curves are presented in Fig. 7.16, demonstrating the mechanical properties of the ITZ to have dominant influence on tensile fracture behaviour of concrete. Improved tensile performance of concrete is resulting from model material with higher mechanical properties for the ITZ. The relationship of peak tensile force of concrete with tensile strength of the ITZ is plotted in Fig. 7.17.

Fig. 7.16 F-D curves of models in which ITZ’s mechanical properties are varied

Fig. 7.17 Peak tensile force of models in which the tensile strength of the ITZ was varied
Figure 7.17 indicates peak the tensile force to gradually increase with increasing tensile strength of the ITZ. High tensile strength of the ITZ will dramatically improve the tensile strength of concrete. However, promoting mechanical properties of the ITZ goes hand in hand with doing so for the matrix normally. This will be the case when reducing w/c. A specific improvement in ITZ density can be obtained by properly designed cement, leading to improved packing density (Bui et al., 2005; Goldman and Bentur, 1995).

### 7.4.6 Influence of mechanical properties of matrix

Similar as ITZ, mechanical properties of the matrix also rely on the technical design parameters and curing conditions. To identify the influence of mechanical properties of matrix on the fracture behaviour of concrete, the structure model as Fig. 7.10 is used for an assessment. Different materials properties are applied to the matrix as different ratios to aggregate shown in Table 7.4. The properties of ITZ are assumed to keep the 0.6 ratio of properties of matrix in case I, while keeping the constant in case II. Therefore, in case I, the results will show influence of mechanical properties of matrix and ITZ on fracture behaviour of concrete. Comparison of results of case two and case I shows the difference in influence of mechanical properties of matrix and ITZ on fracture behaviour of concrete.

<table>
<thead>
<tr>
<th>Ratio of Young’s moduli of aggregate and matrix (E_{agg}/E_{matrix})</th>
<th>E of matrix (E_{matrix}) (MPa)</th>
<th>Tensile strength of matrix (MPa)</th>
<th>E of ITZ (E_{itz}) (MPa)</th>
<th>Tensile strength of ITZ (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.25</td>
<td>12</td>
<td>6</td>
<td>9 (case I)</td>
<td>7.5 (case I)</td>
</tr>
<tr>
<td>5</td>
<td>15</td>
<td>14</td>
<td>7.2 (case II)</td>
<td>2.2 (case II)</td>
</tr>
<tr>
<td>3</td>
<td>25</td>
<td>27</td>
<td>7.2 (case II)</td>
<td>2.2 (case II)</td>
</tr>
<tr>
<td>1</td>
<td>75</td>
<td>40</td>
<td>45 (case I)</td>
<td>21.3 (case I)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>7.2 (case II)</td>
<td>2.2 (case II)</td>
</tr>
</tbody>
</table>

Finally results of F-D curves in different situations are shown in Fig. 7.18. It illustrates that peak force values of concrete are increased dramatically when increasing mechanical properties of matrix and its corresponding ITZ (in case I). But if mechanical properties of ITZ keep constant like in case II, improving mechanical properties of matrix will only increase peak force value in a moderate range. The relationships of peak force value with different mechanical properties of matrix in different cases are shown in Fig. 7.19.

Therefore, compared with influence of mechanical properties of ITZ, sole by changing of mechanical properties of matrix has limited impact on the fracture behaviour of concrete. Mechanical properties of matrix as well as ITZ should both be improved for a better fracture behaviour of concrete.
7 Influence of Particle Packing on Fracture Behaviour of Concrete

Fig. 7.18 F-D curves of models in which mechanical properties of matrix and ITZ are varied

Fig. 7.19 Peak force of models in which mechanical properties of matrix and ITZ are varied (case I: change mechanical properties of matrix and corresponding ITZ; case II: only change mechanical properties of matrix)

7.5 Summary

Fracture behaviour of model concrete was analyzed in this study on meso-scale. Major objective is to investigate the influences of particle shape and of particle packing of aggregate on fracture behaviour of concrete. The results show that particle shape has modest influence on tensile strength of concrete. Models with arbitrary angular shaped inclusions have lower tensile peak force as compared to models with circular aggregate grains. This is due to higher stress concentrations near the aggregate. Packing density of aggregate is another important parameter for tensile fracture behaviour. It seems that a model with higher packing density of aggregate has a lower tensile strength. But these properties are largely influenced by the properties of ITZ. A model with higher packing density of aggregate has a comparable peak tensile force compared with models with lower
concentration of aggregate. It is also found in this study that mechanical properties of aggregate have insignificant influence on fracture behaviour of concrete as long as the aggregate is stronger than the matrix. That implies cracks to be always initiated in the ITZ or in the matrix. ITZ has a dominant influence on tensile fracture behaviour of normal concrete. A larger width of the ITZ will result in a more ductile softening of concrete and in a slightly lower peak force. Mechanical properties of ITZ directly influence the tensile fracture of concrete. A model with higher mechanical properties of ITZ has a better tensile fracture behaviour. Compared with ITZ, higher mechanical properties of matrix will also result in better fracture behaviour of concrete. This phenomenon is more paramount in the case where mechanical properties of ITZ are also changed compared with the case when keeping ITZ's properties stable. This indicates that both improvements of the mechanical properties of the ITZ as well as matrix will yield improved tensile fracture performance of the concrete.
CHAPTER 8

PARTICLE PACKING AND SELF-HEALING OF CEMENT PASTE

Transport of harmful substances through the pore space of concrete can give rise to deterioration of concrete structure or to corrosion of steel reinforcement. Internal and external influences will additionally lead to the formation of myriads of tiny cracks in the virgin state. These cracks can have detrimental impact on concrete durability. Nuclei of cement particles left unhydrated in concrete after maturation can provide under favorable conditions a self-healing capability to micro-cracked concrete. A prerequisite is that the small cracks, for which repair by self-healing is considered, pass through regions containing the unhydrated cement. Such micro-cracks predominantly run through ITZs. Therefore, containers with rigid boundaries as well as periodic boundaries were employed for the production of series of cement paste specimens by a concurrent algorithm-based discrete element computer simulation system with the acronym SPACE. They were subjected to quantitative microstructure analysis of which relevant data on global parameters and on gradient structures in the ITZ are presented and discussed in this chapter in terms of concrete’s possible self-healing capability.

8.1 Introduction

Concrete is a brittle material. Reinforcement is needed when dealing with tension or bending situations. Transport of harmful substances through pore space can give rise to deterioration of concrete structure or to corrosion of steel reinforcement. Hence, geometric and topological studies on the pore space are highly relevant. Shrinkage and local secondary displacements during maturation lead in the virgin state to the formation of myriads of tiny cracks in the concrete’s cement paste, the major part of which will be situated in interphase regions around aggregate grains (Stroeven, 1973). Additional micro-cracks can be initiated, of course, by external influences, such as by freeze-thawing, temperature gradients and mechanical loading. The dispersion of such cracks is inevitably governed by the dispersion of the aggregate grains in the so-called jammed state. These fine cracks can heal under favorable conditions, a phenomenon referred to at least as early as 1937 by Turner (1937) as self-healing or autogenously healing. Several mechanisms of self-healing are proposed (Neville, 1995), i.e., hydration of the hitherto unhydrated cement, formation of insoluble calcium carbonate, and mechanical blocking by very fine material suspended in the water.

This chapter focuses on the first mechanism in a computer simulation approach, whereby the self-healing capability can be expected to be primarily dependent on the amount of unhydrated cement. However, also number density and spacing distribution of unhydrated
cement nuclei (UCN) could play a role, defining it as a configuration-sensitive phenomenon (Stroeven, 1973). The problem that should be tackled concerns the assessment of the (near) intersection frequency of dispersed micro-cracks and dispersed unhydrated cement particles. This chapter will only consider the self-healing capacity of selected crack paths through properly simulated spatial UCN structures. To do so, the simulation system must be capable of dispersing the cement particles “realistically” in the fresh state. This can be achieved by a concurrent algorithm-based system (Stroeven and Stroeven, 1997; Stroeven, 1999).

Concrete is a macroscopically heterogeneous material, requiring elements of macroscopic dimensions to reduce scatter to an acceptable level in the various independent global descriptors of its structure. Such elements define the size of the “homogeneous” representative volume elements (RVEs) in 3D and representative area elements (RAEs) in 2D for successive descriptors. Order of magnitude of the linear dimension of a cube-shaped RVE for composition homogeneity is about four times the maximum grain size (Cook and Seddon, 1956). However, this linear dimension may be an order of magnitude larger when dealing with extreme configuration-sensitivity (Brown, 1965; Stroeven, 1973). The average nearest neighbour aggregate grain surface-to-surface spacing in normal concrete is of the order of 50 μm (Scrivener et al., 2004), in a range of 0.1-200 μm (Chen et al., 2005). Major part of the cement paste will therefore be pocketed between two or more aggregate grains inside ITZs with basically properties deviating from those in bulk. The density is lower, and porosity and connected fraction of porosity are found concentrated inside ITZs (Chen et al., 2006). The relevance of focusing on the ITZ in this chapter is therefore coming from the high probability that a crack will traverse this zone (Jacobsen et al., 1995).

Experimental information seems limited to self-healing effects in concrete elements provided with a single relatively small crack subjected to mechanical loading (Kasperkiewicz and Stroeven, 1991; Granger et al., 2005). Further, only scare experimental evidence is available as to technological influences (such as water to cement ratio, cement fineness, cement type) on the self-healing capacity of concrete (Liu et al., 2005; Heide and Schlangen, 2007).

8.2 Materials

Four different types of Portland cement (PC) are employed in pastes with water to cement ratios (w/c) of 0.2, 0.3, 0.4, 0.5, and 0.6. The PC types are denoted by C164, C206, C319, and C497, whereby the Blaine number defines the specific surface area in m²/kg (i.e., C164 is a cement with Blaine number 164). The respective particle size distribution (PSD) functions comply with the so-called Rosin-Rammler size distribution function (Hu, 2004; Stroeven, 1999; van Breugel, 1997):

\[ G(d) = 1 - \exp(-bd^a) \]  

(8.1)

in which \( a \) and \( b \) are two constants that have to be specified for each cement type and \( d \) is sieve opening size. The cumulative size distribution curves of the model cements are shown in the Fig. 8.1, with grain sizes between 1 and 40.5μm, 1 and 34.7 μm, 1 and 26.2 μm, and 1 and 18.8 μm for C164, C206, C319 and C497, respectively.
8.3 Methodology

As introduced in Chapter 3, the discrete element simulation system SPACE models the fresh paste as a set of spherical elements dispersed in water (Stroeven and Stroeven, 1999). Since these elements represent real physical phases in the material, physical properties can be assigned to each element along with its size. There are two vital stages incorporated in the SPACE system. During the dynamic packing stage, the iteration stops when a certain condition is met, e.g., the relevant volume fraction of particles is reached. Another vital stage is the hydration process. Individual hydrating cement particles are represented by sets of concentric spheres in the early stages of the hydration process. The kinetics of the hydration process is governed in an initial stage by a boundary mechanism, followed by one in which the reaction rate is controlled by a diffusion mechanism. For more detailed information, see Stroeven (1999) or Stroeven and Stroeven (1999). The hydration algorithms largely correspond to those of HYMOISTRUC3D (van Breugel, 1997).

8.4 Experiments

For each specimen, a total number of 5000 cement particles were generated conforming to the four PSDs of Fig. 8.1. After dynamic packing, model cements with final volume fractions of 35%, 39%, 44%, 51% and 61% were obtained, corresponding to w/c of 0.6, 0.5, 0.4, 0.3, and 0.2, respectively. Different boundary conditions are applied for comparison purpose. C164, C319 and C497 are made with periodic boundaries, representing bulk cement paste. C206, C319 and C497 are produced with a rigid boundary condition, yielding paste with ITZs. Each combination of parameters was represented in this study by a single cube. The final linear dimensions of the cubes were in the range 91.1–109.6, 75.7–91.1, 51.3–61.7 and 40.7–49 μm for C164, C206, C319 and C497, respectively. Hence, the cube size is smaller than the RVE (or RAE) for composition. However, the size ratios of cubes and RVEs for composition are relatively similar over the total testing range, as shown in Table 8.1. When it is assumed that the RVE/RAE size for a given configuration-sensitive descriptor is a certain (descriptor-sensitive!) factor exceeding the one for composition homogeneity, an unbiased
Table 8.1  *Ratios of linear dimensions of cubes and RVE for composition homogeneity*

<table>
<thead>
<tr>
<th>Cement</th>
<th>w/c</th>
<th>0.2</th>
<th>0.3</th>
<th>0.4</th>
<th>0.5</th>
<th>0.6</th>
</tr>
</thead>
<tbody>
<tr>
<td>C164</td>
<td>0.57</td>
<td>0.61</td>
<td>0.64</td>
<td>0.67</td>
<td>0.69</td>
<td></td>
</tr>
<tr>
<td>C206</td>
<td>0.55</td>
<td>0.58</td>
<td>0.61</td>
<td>0.63</td>
<td>0.66</td>
<td></td>
</tr>
<tr>
<td>C319</td>
<td>0.49</td>
<td>0.52</td>
<td>0.55</td>
<td>0.57</td>
<td>0.59</td>
<td></td>
</tr>
<tr>
<td>C497</td>
<td>0.54</td>
<td>0.57</td>
<td>0.60</td>
<td>0.63</td>
<td>0.65</td>
<td></td>
</tr>
</tbody>
</table>

*Comparison study* would still be possible (Hu and Stroeven, 2005). At least trends should be considered reliable, therefore, in this preliminary study.

### 8.5 Results

#### 8.5.1 Global results on structure

Models with periodic boundary conditions are hydrated for 1 year. Models with rigid boundaries are hydrated for 28 days and 1 year for comparison purposes. Fig. 8.2 shows a

![Fig. 8.2](image)

*Fig. 8.2 Cement pastes and UCN of C319 with rigid boundaries (a) after 28-days of hydration, (b) after 1 year of hydration, and (c) with periodic boundaries after 1 year of hydration*
selection of the SPACE-generated structures of hardened cement paste and of associated UCN of C319, obtained for different values of \(w/c\), hydration duration and boundary conditions. This information offers a visual perception on the UCN structures as functions of these technological parameters. Due to different packing density or \(w/c\), degrees of hydration are different as reflected by the different amounts of UCN left in the models. Next step is the geometrical statistical (\textit{i.e.}, stereological) description of features of these structures, so that a \textit{comparative} study can be conducted in a quantitative way.

The simplest one is the configuration-insensitive volume fraction descriptor, \(V_v\). Data in Fig. 8.3(a) pertain to the average value of volume density in the cube; they demonstrate the fineness of the cement to have a limited effect on this parameter at equal \(w/c\), especially at low values. The many tiny UCN only marginally influence this parameter. But hydration duration has some effects on this parameter because of different degrees of hydration. Of course, longer hydration duration will result in a higher hydration degree. Hence, as a result, a lower amount of UCN is left after 1 year’s hydration as compared to models at 28-days of hydration.

However, this is different for the average number density in the cube, or the number of nuclei per unit of sample volume, \(N_v\). The sensitivity level was set at 0.01 \(\mu\)m; smaller nuclei are not expected exerting significant effects on the self-healing capacity. Results are presented in Fig. 8.3(b). Paste made by a finer cement has a higher number density of UCN. With longer hydration duration, number density of UCN is also decreased. But this phenomenon is more significant in paste made by finer cement. The differences in degree of hydration are shown in Fig. 8.4(a) with different \(w/c\), fineness and hydration duration for rigid boundary cases. It seems that the degree of hydration at \(w/c=0.2\) is almost similar in models with different fineness of cement and hydration duration. The main cause of this phenomenon is a limitation of water, which controls the hydration. Generally speaking, models made by finer cement have higher degrees of hydration. Longer duration of hydration results in a high degree of hydration. Fig. 8.4(b) indicates surface area density, \(S_v\), to be influenced by the fineness of cement and by \(w/c\) in models with periodic boundary condition and at 1 year’s hydration. It reveals that finer cement has a higher surface area density of UCN. \(S_v\) decreases dramatically with increase of \(w/c\). Similar results are found for

![Fig. 8.3](image-url) (a) *Volume fraction of UCN and (b) number of UCN per unit volume for cements with different \(w/c\) and at different hydration durations*
the pastes with rigid boundary conditions that will be shown later. This parameter is expected being related to self-healing probability, which will be discussed later.

The same sensitivity level was maintained for the highly configuration-sensitive nearest neighbour surface-to-surface spacing (NNSSS). A single example is presented in Fig. 8.5(a) for \( w/c = 0.2 \) at 28-days of hydration with rigid boundaries. Larger cubes would have yielded smoother curves, however, also in shifts in average values. Smoothening can also be achieved by averaging over a series of identical tests, maintaining the shifts of average values. This is common practice in systematic research. These shifts can be compared with so-called “size effects” in fracture mechanics. The RVE/RAE size can be derived from large test series on different sample sizes, from which probability density functions of the desired descriptor are obtained. As stipulated earlier, this was not pursued in this preliminary study.

The different measures for the curve’s characteristic averages are approximately increasing linearly with \( w/c \), as depicted by Fig. 8.5(b). Hence, cement more completely hydrates at higher \( w/c \) and the resulting smaller numbers of nuclei left unhydrated are, as
a consequence, more remote from each other. Similar results were found in models with periodic boundaries after 1 year’s hydration (He et al., 2007).

### 8.5.2 Local results on structure

So far, the ITZ properties are globally characterized in a model with rigid boundaries. They can be compared with global bulk values. Additionally, gradients in local values perpendicular to the aggregate grain’s surface have been determined for UCN, solid gel and porosity. As stipulated earlier, sampled areas are of sub-RAE size. Nevertheless, the volume fraction gradient inside the ITZ is obtained in an unbiased way (accepting somewhat more scatter due to sub-RAE nature of experiments). Fig. 8.6 only shows as an example \(V_V\)-gradients of solid gel and porosity in C497 with rigid boundaries after 28 days’ hydration. Fig. 8.7(a) shows its corresponding gradients of UCN in the pastes.

Gradient structures of UCN, gel and porosity in Fig. 8.6 and 8.7(a), clearly reveal the wall effects in \(V_V\), defining the extent of the ITZ. However, extensions of ITZ vary for different descriptors (Hu and Stroeven, 2004). It seems that the extension of ITZ is about 5 μm from the point of view of solid gel or porosity in Fig. 8.6. Nevertheless, the order of magnitude of the ITZ’s extent for volume fraction of UCN is 10 μm (i.e., only part of maximum grain size), which is estimated from Fig. 8.7(a). This value is slightly increased with \(w/c\), as shown earlier in Stroeven (1999). The fractional volume density of the solid gel or UCN declines from bulk toward the aggregate surface. This is more pronounced for the lower \(w/c\) case. An opposite conclusion can be drawn with respect to porosity. Fig. 8.7(b) presents the same data as Fig. 8.7(a), however comparing the different cement types for the sole case of \(w/c=0.2\). The slope in the gradient structures is the steepest for the fine-grained cement, although leading roughly to a similar level in bulk volume density as earlier shown in Fig. 8.3(a). Hence, low \(w/c\) and high cement fineness basically promote arriving at higher volume densities in the proximity of the aggregate grain surfaces.

With low \(w/c\), Figure 8.3 demonstrated the finer cement to yield far larger global numbers of UCN despite a similar volume fraction. For the same low \(w/c\) after 28 days’ hydration, the gradient in local number density of UCN is depicted in Fig. 8.8(a). It reveals number density increasing from surface of aggregate to a certain level and thereupon declining slowly, revealing a very extensive ITZ (Stroeven, 1999). Finer cement has a high number density of

![Gradient in VV of (a) solid gel and (b) pores in C497 for five values of w/c after 28 days hydration](image)

Fig. 8.6
UCN throughout the whole range conforming to Fig. 8.3(b).

Figure 8.8(b) indicates surface area density, $S_V$, to be influenced by the fineness of cement at the same $w/c$. It reveals finer cement having a high surface area density of UCN. This parameter could be expected to relate to probability of self-healing, which will be discussed later.

The mean free spacing $\lambda$, defined as the mean uninterrupted surface-to-surface distance between all neighbouring particles, is another relevant 3D structure parameter. It can be calculated for the UCN structure by Eq. (8.2) and as a consequence reveals the dependence of surface area density on the technological parameters, as demonstrated in Fig. 8.9(a) for global values of the model hydrated for 1 year; the finer cement specimen has somewhat lower mean free spacing of UCN ($w/c \leq 0.4$). The local gradient structure information is presented in Fig. 8.9(b). Although the mean free spacing of UCN is high close to the aggregate grain’s surface (reflecting high porosity values), it rapidly diminishes to its plateau value at a distance of about 5 $\mu$m. The ITZ thickness seems smallest for the finest cement. The extension of ITZ characterized from $\lambda$ is more close to value expected from solid gel or porosity of pastes in Fig. 8.6.
Fig. 8.9 (a) Mean free spacing $\lambda$ for different types of cement and different w/c and (b) gradients in mean free spacing $\lambda$ for different types of cement (w/c=0.2), both in models after 1 year of hydration.

The radii and geometric distributions of UCN in cement paste models are directly reflected by Fig. 8.10 for C206 and C497 with w/c=0.2 after 1 year of hydration. There is a region in the ITZ where the number of the UCN is exiguous. The distance of this span is about 0.2 $\mu$m for rare number of cement nuclei. Therefore the cracks will have a high probability propagating through this region. This part could be considered “outer” ITZ. “Inner” ITZ will be considered as additional part of ITZ, where the number of UCN is significantly higher than in the outer ITZ although the size of UCN is small. This leads to low values of volume fraction in this region while the number density keeps similar level of bulk. It is reasonable to assume the connectively of pores are gradually decreased from outer ITZ to inner ITZ like the finding by Chen et al. (2006).

8.5.3 Crack healing

To approximately assess crack healing capacity in cement paste, it is assumed that cracks
will be initiated parallel to the aggregate grain’s surface and perpendicular to one reference axis for models with rigid and periodic boundaries, respectively. So, a number of sections are selected to represent cracks in the model paste (see Fig. 8.11). Each single crack is assumed to be independent. Therefore, there are no interactions between cracks. The area fraction of UCN in the crack is a parameter that can be associated in a first order approximation with the self-healing capacity. Unbiased representation of the area fraction is the volume fraction shown in Fig. 8.7 based on a basic stereological relationship \( A_A = V_V \). Prime contribution to self-healing is supposedly coming from all hydrating UCN in cracks, thus ignoring possible contributions due to diffusion through pores of hydration products from more remote UCN (see Fig. 8.12). The maximum width \( W_{\text{max}} \) of healable cracks opening is used as an evaluation index for self-healing capacity. Power’s hydration model is employed to set up the following equations (Jensen and Hansen, 2001).

\[
V_{cs} = 6.410^5 \rho_c (1 - p)\alpha = 0.2(1 - p)\alpha \tag{8.3}
\]

\[
V_{cw} = p - \frac{(0.19 + 0.23)\rho_c (1 - p)\alpha}{\rho_w} = p - 1.32(1 - p)\alpha \tag{8.4}
\]

\[
V_{gw} = \frac{0.19\rho_c (1 - p)\alpha}{\rho_w} = 0.60(1 - p)\alpha \tag{8.5}
\]

\[
V_{gs} = 1 - 6.410^5 \rho_c + \frac{0.23\rho_c (1 - p)\alpha}{\rho_w} = 1.52(1 - p)\alpha \tag{8.6}
\]

\[
V_{scn} = (1 - p)(1 - \alpha) \tag{8.7}
\]

in which,

\[
p = \frac{(w/c)}{(w/c + \rho_w / \rho_c)} \tag{8.8}
\]

**Fig. 8.11** Cracks considered in model cement paste with (a) rigid boundaries and (b) periodic boundaries.
Fig. 8.12 Single crack intersected with cement pastes with (a) rigid and (b) periodic boundaries

\[V_{cs}, V_{cw}, V_{gw}, V_{gs}, V_{ucn}\] are volume fraction resulting from chemical shrinkage of capillary water, of gel water, of gel solid, and of unhydrated cement nuclei, respectively. \(p\) is the initial porosity. \(\alpha\) is the degree of hydration (DOH). \(\rho_c\) and \(\rho_w\) denote the density of cement and water, respectively, with \(\rho_c = 3.15\) g/cm\(^3\) and \(\rho_w = 1.0\) g/cm\(^3\).

The amount of water is assumed sufficient for further hydration of UCN in the crack. The same \(w/c\) as the initial one is also assumed for the default further hydration, so that strength can regain its original level. Therefore, further hydration is assumed happening in the open system with initial \(w/c\). The additional water \(V_{aw}\) can make up for the volume due to chemical shrinkage \(V_{cs}\), despite the degree of hydration \(\alpha\). Therefore, the total amount of reaction productions in the open system can be calculated by

\[V_{rp} = V_{cw} + V_{gw} + V_{gs} + V_{ucn} + V_{aw} = 1\]  

(8.9)

Before hydration of UCN (i.e., \(\alpha = 0\)), the initial fractional volume of UCN is \(V_{ucn_0} = (1 - p)\).

The final volume ratio of reaction products from UCN is:

\[\frac{V_{rp}}{V_{ucn_0}} = \frac{1}{(1 - p)}\]  

(8.10)

The final volume ratio of reaction products coming from UCN is presented in Table 8.2.

<table>
<thead>
<tr>
<th>(w/c)</th>
<th>Initial porosity, (p)</th>
<th>Volume ratio of reaction products from UCN, (\frac{V_{rp}}{V_{ucn_0}})</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2</td>
<td>0.387</td>
<td>1.631</td>
</tr>
<tr>
<td>0.3</td>
<td>0.486</td>
<td>1.946</td>
</tr>
<tr>
<td>0.4</td>
<td>0.558</td>
<td>2.262</td>
</tr>
<tr>
<td>0.5</td>
<td>0.612</td>
<td>2.577</td>
</tr>
<tr>
<td>0.6</td>
<td>0.654</td>
<td>2.890</td>
</tr>
</tbody>
</table>
Therefore, maximum width of crack opening $W_{\text{max}}$ that could be healed by further hydration of UCN can be estimated by Eq. (8.11), in which $A_{\text{crack}}$ is surface area of crack.

$$W_{\text{max}} = \frac{V_p - V_{\text{min}}}{A_{\text{crack}}} \quad (8.11)$$

Figures 8.13(a), 8.13(b) and 8.14(a) present gradient data on maximum healable crack opening in three different types of cement paste with different w/c and rigid boundaries after 28 days hydration. Larger crack openings can be healed in low w/c pastes. This could have been concluded from Figs. 8.3 and 8.5, as well. The maximum width of cracks that can be healed gradually increases away from the surface of aggregate grains, like other relevant parameters do. Values of maximum width of healable cracks are different in cements with different w/c (Fig. 8.14(a)), and with different fineness (Fig. 8.14(b)), all arriving finally at respective bulk values.
8.6 Discussion

Influences are investigated in this chapter exerted by \( w/c \), fineness of cement paste, hydration duration and boundary condition on the structure of cement paste, especially the UCN that is underlying concrete's self-healing capacity.

Volume fractions of UCN are marginally depending on cement fineness, declining at increasing \( w/c \) and hydration duration as depicted by Fig. 8.3(a). Volume fraction of UCN is becoming insignificant for \( w/c \geq 0.4 \), in agreement with Power's model (Jensen and Hansen, 2001). Obviously, the associated high water contents allow for more complete hydration, and, as a consequence, smaller amounts of UCN will be left. Compared to fineness of cement, \( w/c \) is the dominating factor for the self-healing capacity of concrete as additionally shown by Fig. 8.3(a). At higher \( w/c \), in bulk and in ITZ alike, averages of NNSSS of UCN increase;
nuclei are more widely spread.

The cement fineness level has significant impact on the number density of UCN \((N_v)\) within a limited range of \(w/c\), \(i.e., 0.2 \text{ to } 0.4\), as illustrated in Figs. 8.3(b). In this range, the finest cement (C497) reveals much higher number density, which can be attributed to the initially large value of \(N_v\) in the fresh state of the cement. On the other hand, the finer cement leads to lower averages of NNSSS of UCN despite the degree of hydration (DOH) being only slightly different. These results are very similar to those obtained with periodic container boundaries, representing bulk conditions (He et al., 2007).

The ITZ is most liable to crack formation (Stroeven, 1973; Jacobsen et al., 1995). The probability of micro-cracks in these zones to interfere with the UCN can be expected depending as a first order approximation on the volume fraction of UCN. Furthermore, a tendency of cracks to follow the external surface of the UCN was found experimentally (Baldie, 1985; Struble et al., 1989). Baldie explains this phenomenon by conceiving the UCNs as strong inclusions in the hardened cement paste. Therefore, surface area density, \(S_o\) of UCN can additionally be assumed related to concrete’s self-healing capacity. Finer cements were found producing relatively high surface area density in ITZs. As a result, higher second order contributions to self-healing probability can be expected in concretes made by finer cements.

Basically, spacing, size and number of UCN can all be expected vital factors for self-healing capacity of concrete. Although high number and surface area densities are found in finer-grained model cements, self-healing capacity will be limited due to the small size of the UCN (such as in C497), and vice versa. Model cements combining relatively large UCN with high number densities (so, smaller spacing), such as in the case of model cement C319 inside rigid boundaries, could have optimum self-healing capacity pertaining also to larger crack openings. It is also found that coarse cement has a higher capacity of self-healing in bulk paste.

Correlation between the self-healing capacity of concrete and the fineness level of cement was experimentally studied in (Liu et al., 2005). The authors used two types of cement (P.O 32.5 and P.O 42.5, Chinese codes representing coarse and fine cement, respectively) and measured the compression strength of concrete cubes after self-healing experiments. The involved \(w/c\) was 0.358. It can be expected that the strength of concrete made with finer cement revealed higher strength both before and after the self-healing testing. However, the strength ratio of self-healed concrete compared to the matured (and by purpose cracked) concrete cube (before self-healing experiments) was slightly higher in the case of the coarser cement. This ratio is used to describe the self-healing capacity of concrete in (Liu et al., 2005). These results form supporting evidence for our findings.

Heide and Schlangen (2007) investigated experimentally the self-healing effects in early-age cracked concrete. They found that up to 50 \(\mu\)m crack openings imposed in three-point-bending test were closed after certain periods of curing in water. But it was found imposing compressive stress to close cracks during curing was necessary for self-healing of crack in this study. This is supported by the predicted values of maximum healable crack opening in Fig. 8.14(b) or Fig. 8.15(b) of this paper. Self-healing by further hydration of cement is obviously more effective for micro-cracks in concrete. One important thing to remember is that what has been discussed in this paper concerns a theoretical model
concept for self-healing due to UCN. The larger size of cement particles in practice can contribute to additional self-healing capacity. On the other hand, insufficient hydration of UCN found in cracks will reduce self-healing capacity; this process will also be affected by other physical or chemical influences. Therefore, self-healing capacity due to UCN in concrete will be affected by many factors. Certainly, other self-healing mechanisms will additionally contribute to its capacity in practice, which have not been discussed here.

8.7 Summary

A mixture of composition and configuration-sensitive descriptors of material structure can provide reliable quantitative information on the evolution process of UCN during maturation of a range of cement pastes. This can be achieved by concurrent algorithm-based computer simulated systems, like SPACE.

The results show that the extension of ITZ is not only influenced by the technical parameters such as w/c, fineness of cement, duration of hydration, etc., but also depend on the parameters used for characterization.

The water to cement ratio (w/c) is a key factor for self-healing capacity of hardened concrete. For $w/c \geq 0.4$, the amount of UCN is limited. Hence, discussion on self-healing capacity of concrete is only more sensible for a limited, but for HPC relevant range of $w/c$ ($w/c \leq 0.4$) after maturation.

Concrete made with finer cement has higher surface area and number density of UCN (even higher in ITZs) for given $w/c$, so that relatively high probability of self-healing is expected for such types of concrete. But optimum self-healing capacity, which also involves healing of larger crack openings, can only be expected in model cements combining larger size UCN, dense distribution and high number density of UCN.

Self-healing capacity due to UCN in concrete is expected to be more effective for micro-cracks.
CHAPTER 9

CONCLUSIONS AND RECOMMENDATIONS

9.1 Conclusions

This thesis aimed at developing strategies for simulation of arbitrary shaped particles and their integration in a DEM-based particle packing system. Upon realization of this goal, this DEM-based approach proved an efficient tool for studying packing of aggregate or of cement-like particles. More specifically, this approach renders the possibility of conceiving effects exerted by grain size and shape as well as the packing method on structure formation. It can also be conceived an effective approach to modelling of composite particulate materials like the cementitious materials.

Particle shape was found sorting major effects on features of the packed particle structure of the material, among which packing density. Particles of polyhedral shape with higher sphericity tend to yield higher packing density. On the contrary, packing density of particles with elliptic (in 2D) or ellipsoidal shape (in 3D) attained their highest density at relatively low sphericity values. Hereby, sphericity measures how much the particle’s shape deviates from spherical. The coordination number of the packed structure is related to packing density as well as to particle shape. The packing method also influences the final density. Packing with compaction leads to higher densities than is achieved by loose random packing, and coordination numbers are modified accordingly. However, in addition to the proper packing approach, a good combination of particle shape and particle size distribution is necessary for optimum mix design. Analytical methods can reasonable well predict global properties. However, DEM-based packing simulation can reveal more easily and in a visual way effects sorted by various parameters.

Particle packing density has a dominant influence on the elastic properties of concrete as evaluated in a study focusing on numerical concrete on meso-level. Particle shape has limited influence on the elastic properties of concrete. Elastic properties seem to be relatively structure-insensitive. As a consequence, modelling can be based on spherical aggregate for the prediction of elastic properties. The Young’s modulus largely depends on the prime components of concrete such as aggregate and matrix. However, Poisson’s ratio is also sensitive to components with low volume content such as ITZs.

Fracture behaviour of concrete is also significantly influenced by packing of the particles. Particle shape exerts more influence on fracture behaviour than on the elastic properties of the concrete. Models with angular shaped aggregate have lower ultimate tensile strength than those with spherical inclusions. Models of normal concrete with higher aggregate packing density reveal lower ultimate tensile strength. But this phenomenon largely depends on the properties of the ITZs. It is well-known that fracture behaviour of concrete is
governed first of all by weak parts of the concrete such as in the matrix or the ITZ, whereby the latter is the dominant factor. This indicates that improvement of the mechanical properties of the ITZ as well as of the matrix will yield improved tensile fracture performance of the concrete.

The properties of the cement paste rely on the mixed materials and on curing conditions. Properties of ITZ are influenced by technical design parameters such as water to cement ratio (packing density of the cement) and fineness of the cement. Width of the ITZ varies among different parameters characterizing ITZ’s structure. Nevertheless, a paste with lower w/c (higher packing density) or made with finer cement particles leads in concrete generally to an ITZ of smaller extent.

The w/c is the key factor that governs the amount of unhydrated cement in matured concrete, which provides under favourite conditions self-healing capacity to microcracks in concrete influencing fracture behaviour of the concrete. Specifically, a lower w/c leads to a higher self-healing capacity, since a larger amount of unhydrated cement is left after maturation. A matured paste made with finer cement contains unhydrated cement particles with a higher surface area density and larger number density for a given w/c. As a result, a higher self-healing capacity can be expected in this kind of concrete. Of course, optimum self-healing capacity can be expect for model cement paste with unhydrated cement particles of large size, dense distribution and high number density. Lower w/c, shorter curing time, relatively courser cement and enough water supplies can lead to an optimized self-healing capacity. Anyhow, a range of maximum healable crack openings extends in the microcrack range.

9.2 Recommendations

The numerical simulation approach to DEM-based particle packing on different structural levels of concrete has been demonstrated in this study having promising perspectives as to mixture design, optimization and simulation of composite structures of concrete. However, still many aspects are remaining for future research.

The simulation of arbitrary shaped particles can be further refined based on findings of various methods, such as stereoscopic image analysis (as introduced in Chapter 2) and computer tomography. It is recommended that shape analysis and reconstruction simulation should be integrated. For instance, in the simulation of cement grains in Chapter 2, shape analysis results obtained by the X-ray tomography have been used as fundamental information and controlling criterion for the simulation. The surface area of aggregate is of importance as it is linked up with the ITZ properties in concrete. This property depends on the size and the shape of aggregate grains. Simplified simulation schemes for particles can already offer valuable practical information of real concrete. For instance, ellipsoids instead of the traditional spheres can be used to represent aggregate in packing simulations aiming the estimation of volume fraction of ITZ in concrete (Zheng et al., 2009). But deviations in aggregate surface area at given volume fraction will induce biases in the information on ITZ’s volume fraction, which is but a composition parameter. This will hold even stronger for configuration-sensitive characteristics of material structure and the structure-sensitive properties relying on it. A potentially intriguing field of research is porosimetry; the ITZ plays also in this case a crucial role (Chen et al., 2006). As an example, pore topology
required in pore network analysis (Vogel and Roth, 2001; Hu and Stroeven, 2005) requires proper information on overlap of neighbouring ITZs; a configuration sensitive parameter. Shape analysis in future research is expected to reveal more information on such aspects. An example is the information presented by Garboczi and Bullard (2004) on cement grains obtained by μCT. CT, SIA and stereological methods are recommended to be included in experimental methodologies.

The DEM-based approach is an efficient way of packing arbitrary shaped particles such as those in concrete. However, it is still laying a high demand on computer time. Normally, using higher amounts of particles (say, around 1 million) would be of interest to concrete researchers. This is a challenge for this DEM-based packing method. Therefore, further improvements on efficiency should be accomplished. Efforts are recommended to focus on different aspects. For example, the contact detection process could be simplified based on the real situation in dense packing of aggregate. Geometrical judgment could be introduced for this aspect to partly replace some complicated mechanical integration procedures. The application of the encapsulated model based on the Monte Carlo method (introduced in Chapter 3) can also improve packing efficiency. Extensions of the Monte Carlo-based RSA model to ellipsoidal shapes could help improving the initial stage packing density at reduced computer demands. Furthermore, parallel computing methods are demonstrated an efficient approach to large complex calculation schemes (Almasi and Gottlieb, 1989). This provides also a promising measure for improvement of calculation efficiency.

The hydration model of cement plays an important role in microstructure simulation and in property prediction for hardened cement paste. The shape of cement grains has been found to be of importance for hydration and microstructure formation by Bullard and Garboczi (2004). Simulation strategies for cement grains and implementation in a DEM-based model has been developed and discussed in this study (in Chapter 2). This approach renders the possibility of incorporation of more important shape information of real cement than just size. A further refined hydration simulation system is expected to be developed based on this study. Comparison studies could be conducted to verify the improvements of this very approach compared with traditional systems based on the assumption of spherical cement grains in RSA systems. Some stereological theories could be used too for handling complex geometric 3D assessment approaches, like in the examples of Chapter 4 in this study.

Fracture behaviour considered in this study is under tensile loading. It is shown that packing density of the aggregate influences the geometric features of the ITZ, and so has impact on the tensile behaviour of concrete. But this is a property which largely relies on the mechanical properties of the ITZ. It can be expected that also other loading situations, such as compression, bending, etc., will be approached with the developed methodology. The damage model should further be extended to fit the conditions under such conditions. Other methods such as DEM can also be applied in the fracture simulation, like the work concluded by Jing and Stepahansson (2007) in rock engineering.

The ITZ region is found to have significant impact on the fracture behaviour and strength of concrete in this study. Influence of cement blending or of the addition of (very) fine fillers as in self-compacting concrete on the ITZ and on the mechanical properties can be further investigated by experimental and numerical methods.
Self-healing of concrete is an interesting topic for concrete researchers and would be for concrete practice. One of the basic mechanisms is crack healing by rehydration of unhydrated cement left in the matured concrete. This is verified and effects exerted by different technological parameters were estimated in this study (see Chapter 8). Some new experiments (Qian et al., 2009) show its potential usage for concrete. Additional research on this topic is foreseen to conceive fracture of cement or concrete in combination with the self-healing capacity prediction model as developed in this study. Multi-scale simulation approaches are to be preferred in this case.
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SUMMARY

Physical particle packing is becoming a hot topic in concrete technology as more and more types of granular materials are used in concrete either for ecological or for engineering purposes. Although various analytical methods have been developed for optimum mixture design, comprehensive information on particle packing properties is still missing, e.g. on the impact of the packing method on such properties. Computer simulation therefore provides a promising perspective for particle packing simulation. However, developing flexible algorithms for simulation of arbitrary shaped particle packing still remains a challenge for concrete researches.

This study aim offers a solution for these problems. The strategy of simulating particles of arbitrary shape is based on an experimental approach to this problem. The simulation strategies are thereupon implemented into a DEM-based dynamic concurrent algorithm-based simulation (CAS) approach for particle packing. Finally, influences of particle shape, particle size and packing method on packing density are evaluated and discussed.

This methodology renders the possibility of producing virtual concrete on meso-level. In combination with FEM, the influence of particle packing on mechanical properties of concrete has been assessed in this way. In the same way the simulation of cement particle packing can be realized on micro-level. Upon simulation of hydration, the capacity of self-healing of cracks due to unhydrated cement is assessed by a DEM-based simulation system for different cement types and packing densities.

1. Modelling of particle packing and properties assessment

Shape analysis of particles in concrete is discussed in the framework of an experimental approach. The relevant methods of conventional image analysis (IA) and stereoscopic image analysis (SIA) can be considered proper compromises between accuracy and sophistication of equipment. In this study, a gravel sample has been investigated by the conventional IA method. The results confirm the sieve curve not to properly reflect particle size. With the length of the three main axes located in three different scatter bands, only the median one was found to correlate closely to the sieve size. This detailed information is not reflected by other shape parameters specified in the open literature, which basically combine information on the main axes. This approach led to the conclusion of equidimensional particles, a conclusion supported by results of Barksdale and Itani (1994).

A simulation strategy is proposed that would specifically attune to the origin of arbitrary-shaped aggregate. Surface texture simulation can also be considered by this method. This flexible simulation strategy shall be based on relevant image analysis data. These image analysis data can serve to conduct 2D as well as 3D simulations. A study specifically focuses on the simulation of cement grains, pursuing the assessment of physically more realistic shapes as compared to the commonly employed spherical one.
This study encompasses polyhedra and ellipsoids. Experiments by X-ray micro-tomography on real cement served as reference. It has been shown that a limited variation of octahedrons or flat ellipsoids can offer optimum solutions. They offer more realistic S/V-relationships as spheres, which is crucial for cement hydration (Bullard and Garboczi, 2006).

Different algorithm-based approaches to particle packing simulation are then reviewed. A distinction is made between two major groups of packing systems. The first group encompasses random sequential additional (RSA) based packing systems in which particles of diminishing size are successively randomly generated. DEM systems are in the second group. RSA systems are more effective for multi-size particle packing at relatively low particle density. Limitations and possible improvements are also discussed and consequences for particle packing demonstrated by examples. Reliability of the DEM-based system SPACE is validated on the basis of experimental data, involving maximum packing densities. Even properties of structure-sensitive nature can be investigated, which is impossible by RSA systems. Possible applications are evaluated of RSA procedures in DEM systems for packing of arbitrary shaped particle packing. At least, RSA seems effective for simulating the distribution of particles at low densities that can form the initial stage in a CAS system.

A DEM based CAS system, i.e. HADES, is employed for packing simulation of arbitrary shaped particles. The underlying packing algorithms of this approach are introduced and discussed. A physical approach is developed for assessment of mass properties of an arbitrary shaped particle, which is crucial for motion calculation in the dynamic DEM system. This input data are necessary for simulating dynamic behavior of the particles at increasing density. Stereological principles are employed for assessment of particle overlap during this densification process. This so-called dynamic DEM system is used for investigating the influences exerted by particle shape as well as packing method on packed particle structure.

Some simulation results of packed ellipses in 2D reveal shape parameters, such as elongation and circularity, to have significant influence on particle packing. This is confirmed by 3D packing simulations of ellipsoids (Williams and Philipse, 2003), whereby ellipses with small elongation yielded higher packing density than could be realized with spheres (and circles in 2D). On the contrary, packing of ellipses with large elongation or lower circularity yielded lower density than obtained with circles. This research additionally allows drawing the conclusion that circularity seems a better parameter than elongation for describing the influence of shape on packing characteristics. Compaction is also found an effective way for densification of the loose packed particle structure.

Packing simulation results with 3D polyhedra both in the loose as well as the dense random state demonstrate that shape exerts a significant influence on packing density. Polyhedra with large sphericity tend to higher packing densities except for some special shapes such as in the case of dense packed cubes. Average coordination number is shown a sensitive parameter for revealing influences exerted by packing density as well as by particle shape. Compaction leads to an increase in average coordination number.

The study continues by evaluating the influences exerted by particle size on particle packing. A simple theoretical model is employed for predicting this effect, ultimately allowing for optimum mixture design. A numerical approach by an RSA system is then used
for packing simulation. The analytical approach as well as the simulation method is first of all applied to a bimodal mixture and thereupon to a ternary one. The results by the RSA system are found complying with those of the analytical approach. This analytical approach can therefore be used for approximate design of particle mixtures; particle shape, interactions between particles and boundary conditions are neglected however. This approach reveals that addition of fine particles to a mono-sized particle structure is an effective way to improve packing density. Simulations by the DEM approach in 2D space show, however, that such filler effects can be overruled by those due to crystallization. In other words, the interaction between particles can be the dominant factor for packing density in some cases. This phenomenon is outside the scope of RSA systems. More irregular shapes give rise to a reduced effect of crystallization and more significant influence by fillers.

Multi-size particle packing should consider the information obtained from packing of mono-sized particles (or from bi- or tri-modal mixtures) as in de Larrard’s models (de Larrard, 1999). This also allows considering the influence of particle shape. In a DEM approach, influences by particle shape as well as size can be considered in a similar way.

2. Particle packing related material properties

A meso-scale numerical model is used to analyze the elastic properties of normal concrete. Both, angular-shaped as well as circular-shaped aggregates were used to assess influences on elastic properties. The Young’s modulus is found to increase at higher area fraction of aggregate and improved mechanical properties of aggregate, matrix, and ITZ. But the Young's modulus declines with increased extent of the ITZ and at higher water to cement ratio. Poisson's ratio decreases at higher area fraction of aggregate and improved mechanical properties of the ITZ and matrix. Contrary, Poisson’s ratio increases due to a larger extent of the ITZ, a higher water to cement ratio and improved mechanical properties of the aggregate. Furthermore, Poisson’s ratio is found more sensitive than the Young’s modulus for effects exerted by the ITZ. The general conclusion is drawn that reliable estimates of the elastic properties of concrete can be derived from numerical and analytical models based on spherical grain shape, since grain shape only sorts minor influences.

Fracture behaviour of model concrete is also analyzed on meso-scale, whereby particle shape and packing are the major parameters. The results show particle shape to have only a modest influence on tensile strength of concrete. Model concrete with arbitrary angular-shaped inclusions has a lower tensile strength as compared to model concrete with circular aggregate grains. Moreover, a higher packing density of the aggregate yields also a lower tensile strength. However, this observed behaviour strongly depends on properties of the ITZ. It is found in this study that mechanical properties of aggregate have an insignificant influence on fracture behaviour of concrete as long as the aggregate is stronger than the matrix. Crack initiation in this normal-strength concrete takes place in the ITZ, which has a dominant influence on tensile fracture behaviour of concrete. A larger extension of the ITZ will result in a more ductile softening of concrete and in a slightly lower peak force. By improving the mechanical properties of ITZ, fracture behaviour is improved. This also holds for improved properties of the matrix. The tensile strength is therefore more increased when both ITZ and matrix of the concrete are improved.
A mixture of composition and configuration-sensitive descriptors of material structure can provide reliable quantitative information on the evolution process of unhydrated cement nuclei (UCN) during maturation of a range of cement pastes. This has been investigated by the aforementioned SPACE system for a series of cements with different fineness. The results show that the width of ITZ is not only influenced by parameters such as w/c, fineness of cement, duration of hydration, etc, but also depend on the descriptive parameters used for characterization. The water to cement ratio (w/c) is a key factor for the self-healing capacity of hardened concrete. For w/c≥0.4, the amount of UCN is limited. Hence, discussion on the self-healing capacity of matured concrete is only sensible for a limited, but for HPC relevant, range of w/c (w/c≥0.4). Concrete made with finer cement has higher surface area and number density of UCN (even higher in ITZs) for given w/c, so that relatively high probability of self-healing is expected for such types of concrete. But optimum self-healing capacity, which also involves healing of larger crack openings, can only be expected in such model cement pastes in which after maturation larger size UCN are found in larger numbers. It is shown that a cement of moderate coarseness leads to optimized self-healing capacity in the ITZs, whereas for bulk properties the coarsest cement is required. Conditions of maturation (specifically duration) and of rehydration are also important factors governing self-healing capacity of concrete. Younger concrete has a higher self-healing capacity due to higher amount UCN left for rehydration. Sufficient water is necessary for full exploitation of this capacity. Nevertheless, it must be clear that the self-healing capacity of concrete is more effective for micro-cracks. This study reveals maximum crack openings that can be healed are limited to several tens of micrometers. This is supported by recently published experimental data (Qian et al., 2009).
SAMENVATTING

Naar de mate waarin meer soorten korrelachtige componenten voor ecologische of technische doeleinden in beton zullen worden toegepast zal de populariteit binnen de betontechnologie van een fenomeen als deeltjespakking toenemen. Hoewel een aantal analytische methoden voor het voorspellen van pakkingdichtheid is ontwikkeld, is het nog steeds niet mogelijk meer gedetailleerde informatie te verkrijgen, zoals effecten gesorteerd door de pakkingmethode zelf. Computersimulatie biedt daarom een veelbelovend perspectief voor onderzoek aan deeltjespakkingen. Niettemin vormt de ontwikkeling van flexibele algoritmen voor het simuleren van dergelijke pakkingen van deeltjes met willekeurige vorm nog steeds een uitdaging voor betononderzoekers.

De onderhavige studie biedt een oplossing voor deze problematiek. Strategieën die zijn uitgewerkt voor de simulatie van deze deeltjes zijn gebaseerd op experimentele benaderingen van het probleem. Daarna zijn deze strategieën ingebouwd in een DEM systeem dat gebruik maakt van een dynamisch mechanisme van fysieke interactie van korrels. Vervolgens zijn daarmede invloeden van korrelvorm, korrelgrootte en pakkingmethode op de pakkingdichtheid gecodeerd.

Deze methodologie maakt het mogelijk virtueel beton op mesoniveau te realiseren. In combinatie met een eindige elementenmethode is daarom via deze weg het effect van pakkingkarakteristieken op mechanische eigenschappen onderzocht. Ook kan evenzo de simulatie van verscheidene cementspecie op microniveau gerealiseerd worden. Na simulatie van deeltjespakkingen is vervolgens het zelfhelend vermogen van de cementpasta na microscheurvorming onderzocht voor verschillende soorten en pakkingdichtheden van cement.

1. Deeltjespakking: modellering en evaluatie

De evaluatie van de vorm van deeltjes op basis van een experimentele benadering wordt in deze studie besproken. De gebruikte methoden van gewone en van stereoscopische beeldanalyse kunnen gezien worden als een goed compromis wat betreft nauwkeurigheid en geavanceerdheid van de benodigde apparatuur. Een grindmonster is in deze studie met behulp van gewone beeldanalyse onderzocht. De resultaten bevestigen dat de zeefkromme niet een goede weerspiegeling is van de grootte van deeltjes. Slechts de middelste hoofdassen correleerde met de zeefkromme. De lengten van de drie hoofdassen vertoonden een spreiding in drie afzonderlijke banden; een genuanceerd beeld dat niet direct werd weerspiegeld door andere in de literatuur gespecificeerde vormparameters, waarbij in principe combinaties van de drie hoofdassen een rol spelen. Hieruit viel te concluderen dat deeltjes een grote mate van bolvorm (“sphericity”) zouden vertonen; een constatering die overeenkomt met resultaten van Barksdale and Itani (1994).

Er wordt voorgesteld een simulatiestrategie te hanteren die specifiek is voor de
Computational Modelling of Particle Packing in Concrete: Samenvatting

oorsprong van deeltjes met willekeurige vorm. Simulatie van oppervlaktetextuur kan ook in deze strategie worden opgenomen. Een flexibele simulatiestrategie wordt voorgesteld die gebaseerd is op kwantitatieve beeldanalyseresultaten. Deze beeldanalyseresultaten van betrokken deeltjes kunnen dienen voor zowel 2D als 3D simulaties. Een specifieke studie concentreert zich op cementkorrels, waarbij naar meer realistische vormoplossingen is gezocht dan die van de gebruikelijke bol. Deze studie omvatte veelvlakken en ellipsoiden. Experimentele resultaten die werden verkregen door een cementmonster te onderwerpen aan Röntgen-microtomografie zijn daarbij als referentie gebruikt. Er is aangetoond dat optimale oplossingen kunnen worden bereikt door een beperkte variatie aan veelvlakken of aan afgeplatte ellipsoiden te kiezen. Hiermede zijn meer realistische waarden voor de verhouding oppervlakte versus volume (S/V) te genereren dan in het geval van bolvormige deeltjes, wat van cruciaal belang is voor cementhydratatie (Bullard and Garboczi, 2006).

Verschillende simulatiesystemen voor deeltjespakking zijn aan een kritische analyse onderworpen. Hierbij is onderscheid gemaakt tussen twee groepen systemen. De eerste groep omvat systemen waarbij korrels van afnemende grootte willekeurig worden gegenereerd (“RSA-based systems”), terwijl de tweede groep DEM systemen omvat. De onderliggende algoritmen zijn vergeleken en op hun merites getoetst. RSA systemen zijn effectiever wanneer een beperkte pakkingdichtheid van een korrelmengsel met een breed scala aan korrelgrootten moet worden gerealiseerd. Inherente beperkingen en mogelijke verbeteringen worden besproken en gead- strueerd met behulp van voorbeelden. De betrouwbaarheid van het DEM systeem SPACE is gevalideerd aan de hand van experimentele resultaten waarbij maximale pakkingdichthen waren betrokken. Zelfs structuurgevoelige eigenschappen kunnen worden onderzocht, wat onmogelijk is met een RSA systeem. Mogelijke toepassingsmethoden van RSA procedures in DEM systemen voor deeltjespakking zijn geanalyseerd. RSA lijkt daarbij ten minste een efficiënte methode om de initiële deeltjesverdeling met beperkte dichtheid als startsituatie voor een DEM simulatie te beschrijven. Pas in dat laatste pakkingstadium is de interactie van deeltjes essentieel.

Een DEM systeem gebaseerd op interactie van deeltjes is HADES; dit is toegepast voor de pakkingssimulatie van deeltjes met een willekeurige vorm. De onderliggende pakkingalgoritmen zijn geïntroduceerd en besproken. De bepaling van de massa-eigenschappen van dergelijke deeltjes van willekeurig vorm is uitgewerkt. Deze invoergegevens zijn nodig voor het simuleren van het dynamisch gedrag van de deeltjes bij toenemende dichtheid. Stereologische principes zijn gebruikt bij de evaluatie van deeltjesoverlap tijdens dit verdichtingproces. Dit zogenaamde dynamische DEM systeem is toegepast voor onderzoek naar effecten van korrelvorm en verdichtingmethode op de materiaalstructuur; verkregen resultaten zijn gerapporteerd en geanalyseerd.

In de 2D benadering op basis van de dynamische DEM pakking van ellipsen werd aangetoond dat korrelvormparameters zoals slankheid (“elongation”) en cirkelvormigheid (“circularity”) een belangrijke invloed uitoefenden op de pakkingdichtheid. Dit werd bevestigd in de 3D simulatie van ellipsoiden (Williams and Philipse, 2003), waarbij dichtere pakkingen konden worden verkregen met ellipsoiden van beperkte slankheid dan met bollen kon worden gerealiseerd. Een grote slankheid (of lagere cirkelvormigheid) in de 2D benadering leidde echter tot een lagere dichtheid dan met cirkels bereikbaar was. Uit dit onderzoek kan daarnaast worden geconcludeerd dat (de graad van) cirkelvormigheid een
beter criterium lijkt (dan slankheid) bij het definiëren van het effect van korrelvorm op pakkingdichtheid. Eveneens werd duidelijk dat samendrukken een effectieve methode is voor verdichting van een losgepakte deeltjesstructuur.

Pakkingsresultaten verkregen met 3D veelvlakken in los- zowel als dichtgepakte toestand laten eveneens de duidelijke invloed zien van korrelvorm op pakking- dichtheid. Daarbij is een tendens merkbaar dat bij grotere bolvormigheid ("sphericity") een grotere pakkingdichtheid kan worden bereikt. Een uitzondering hierop vormen gepakte deeltjes in de vorm van kubussen. Het gemiddelde coördinatienummer ("coordinate number") is een gevoelige parameter om pakkingdichtheid en de invloed daarop van korrelvorm te registreren. Samendrukken leidt tot toename in deze beschrijvingsparameter van de materiaalstructuur.

Vervolgens is de invloed van korrelgrootte op de eigenschappen van de korrel- pakking bestudeerd. Een eenvoudig analytisch model is daarbij ontwikkeld om deze invloed te kunnen voorspellen, zodat een optimaal korrelmengsel zou kunnen worden ontworpen. Pakkingsimulatie is vervolgens gerealiseerd met een RSA methode. Het analytische model zowel als de simulatiemethode zijn in eerste instantie toegepast op een mengsel van twee verschillende korrelgrootten, daarna is een diervoudig mengsel gekozen. Resultaten van de analytische benadering en van de simulatie bleken vergelijkbaar. Daarom kan deze analytische benadering gebruikt worden voor het bij benadering ontwerpen van optimale korrelmengsels; korrelvorm korrelinteracties en randvoorwaarden blijven daarbij buiten beschouwing. Deze benadering laat zien dat het toevoegen van relatief fijkkorrelig materiaal aan een mengsel van korrels van gelijke grootte een effectieve methode tot dichtheid-vergroting is. De 2D simulatieresultaten met DEM laten overigens zien dat het effect van dergelijke toevoegingen van fijn materiaal kan worden overtroffen door die van het zgn. kristallisatiefenomeen. Kortom, de interactie tussen deeltjes kan de dominante factor zijn die in bepaalde gevallen de pakkingdichtheid bepaalt. Dit ligt buiten bereik van RSA systemen. Bij toenemende onregelmatigheid in korrelvorm neemt het effect van kristallisatie overigens af.

Een analytische benadering van korrelmengsels met een range aan korrelgrootten dient voort te bouwen op de informatie van eenvoudige, tweevoudige of drievoudige korrelmengsels (zoals eerder aangegeven), zoals ook geschiedt in de benadering van de Larrard (1999). Daarbij kan ook het effect van korrelvorm worden meegenomen. In een DEM benadering kan op overeenkomstige wijze worden gehandeld.

2. Deeltjespakking-afhankelijke eigenschappen

Een numeriek model op mesoniveau is gebruikt om de elastische eigenschappen van normale-sterkte beton te analyseren. Zowel hoekig als afgerond materiaal is gebruikt voor dit doel. De elasticiteitsconstante bleek verhoogd te worden door een toename van de toeslagfractie en bij toename in de mechanische eigenschappen van alle componenten (toeslag, matrix en grenszone ("ITZ")). Een daling trad op bij een meer omvangrijker aandeel van de ITZ en bij hogere water/cement-factor. De Poissonconstante daalde bij een toename van de aggregaatfractie en bij toename in de mechanische eigen schappen van matrix en ITZ. Daarentegen leidde een meer uitgebreide ITZ, een hogere water/cement-factor en een
Computational Modelling of Particle Packing in Concrete

Samenvatting

toename in de mechanische eigenschappen van het toeslagmateriaal tot een toename in de Poissonconstant. Bovendien bleek de Poissonconstante meer gevoelig dan de elasticiteitsconstante voor diktevariaties in de ITZ. De algemene conclusie is getrokken dat betrouwbare schattingen van de elastische eigenschappen van beton kunnen worden verkregen met modellen gebaseerd op bolvormige toeslagkorrels, omdat korrelvorm maar een zeer beperkte invloed bleek te sorteren.

Het breukgedrag van modelbeton is ook op meso-niveau beschouwd, waarbij korrelvorm en korrelpakking de voornaamste parameters zijn. Van de korrelvorm is daarbij aangetoond dat slechts een beperkte invloed wordt uitgeoefend op de trek- sterke van beton. Modelbeton met hoekige toeslagkorrels leidt tot een lagere trek- sterke dan bij modelbeton met een zelfde hoeveelheid cirkelvormige toeslagkorrels werd gevonden. Verhoogde dichtheid van de toeslagpakking leidt eveneens tot verlaging van de treksterke. Maar deze eigenschappen hangen in sterke mate af van die van de ITZ. Ook de mechanische eigenschappen van de toeslagkorrels bleken geen duidelijk effect te sorteren op de treksterkte, vooropgezet dat het toeslagmateriaal sterker is dan de matrix. In dit normale-sterkte beton vindt scheurinitiatie plaats in de ITZ. Deze heeft daarom een dominante invloed op de treksterkte-eigenschappen van beton. Een meer uitgebreide ITZ zal daarom leiden tot een wat lagere treksterkte en een vergrote deformatiecapaciteit. Verbeterde mechanische eigenschappen van de ITZ bevorderen de breukeigenschappen van beton direct. Dat geldt overigens ook voor verbeterde eigenschappen van de matrix. Het effect op het breukgedrag is daarom duidelijker wanneer zowel de ITZ als de matrix van beton een verbetering ondergaan.

Een combinatie van structuurbeschrijvende parameters van compositie en opbouwgevoelige aard kan betrouwbare kwantitatieve informatie leveren met betrekking tot de ontwikkeling in het ongehydrateerde cement gedurende veroudering van beton. Dit is onderzocht met behulp van het eerder genoemde SPACE systeem voor een aantal cementen met verschillende fijnheid. De resultaten demonteren dat de dikte van de ITZ niet alleen afhangt van parameters zoals $w/c$-factor, cementfijnheid, hydratatiegraad, enz., maar ook van het type beschrijvende parameter. De $w/c$-factor is de belangrijkste factor die het zelfhelend vermogen van beton bepaalt. Bij hogere $w/c$-factoren ($w/c\leq0.4$) is dit vermogen zeer beperkt. De discussie over het zelfhelend vermogen beperkt zich daarom tot de range van lagere $w/c$-facoren die relevant zijn voor hoge-sterke beton (HPC). Beton gemaakt met een meer fijnkorrelige cement leidt tot een vergroting in aantal en specifieke oppervlak van de ongehydrateerde cementkorrels bij eenzelfde $w/c$-factor. Hier lijkt dus een verhoogd zelfhelend vermogen verwacht te kunnen worden. Maar een optimale situatie, waarbij ook aan scheurtjes met grotere scheuropening gedacht moet worden, vereist dat grotere korrels ongehydrateerde cement in voldoende dichtheid aanwezig zullen zijn. Het onderzoek laat zien dat een wat grofkorrelig cement tot optimaal zelfhelend vermogen leidt in de ITZ, terwijl dit in de matrix pas het geval is voor het meest grofkorrelige cement. Omstandigheden bij verharding en gedurende het zelfhelingsproces zijn echter eveneens zeer belangrijk. Jong beton heeft een groter zelfhelend vermogen vanwege de grotere hoeveelheid ongehydrateerde cement. Voldoende water is nodig om het zelfhelend vermogen geheel te kunnen exploiteren. Niettemin mag het duidelijk zijn dat dit vermogen van beton vooral effectief zal zijn bij microscheurtjes. In deze studie is gevonden dat
maximale scheuropeningen die nog tot zelfheling leiden slechts een aantal tientallen micrometers kunnen bedragen. Dit wordt ondersteund door recent gepubliceerd experimenteel materiaal (Qian et al., 2009).

(Dutch translation by Piet Stroeven)
RELEVANT PUBLICATIONS


de Schutter (Eds.), *Concrete Modelling; CONMOD ’08*. Bagneux: Rilem, 479-486.


PROPOSITIONS

1. Particle interference is fundamental in realistically simulating concrete's aggregate or pocketed cement dispersion.

2. Concrete heterogeneity is a sampling and not a material property, although the latter concept is supported by a vast majority of concrete technologists.

3. The autogenous healing capacity of normal concrete requires proper cement, as in the Chinese saying: “The best housewife can't cook a meal without rice”.

4. Concrete facts about concrete are more and more found in virtual reality.

5. Numerical simulation aims at enhancing insight not just at mimicking nature.

6. Good preparation is half the job.

7. Success is associated with the persistence to make another step.

8. Limited knowledge manifests itself by the inability to formulate questions.

9. Many drops fill out the sea.

10. It is always of prime importance for a researcher to find out the principal contradictions in an issue.

These propositions are considered opposable and defendable and as such have been approved by the supervisor Prof.dr.ir. L.J. Sluys.
STELLINGEN

1. Interactie van deeltjes is van fundamentele betekenis voor het realistisch simuleren van verdelingen van toeslagkorrels of van door deze toeslagkorrels ingesloten cementdeeltjes in beton.

2. Heterogeniteit van beton is een bemonstering- en niet een materiaaleigenschap, hoewel een overgroot deel van de betontechnologen dat laatste idee aanhangt.

3. Voor het zelfherstellend vermogen van beton is een geschikt cement vereist, zoals ook in het Chinese gezegde wordt verwoord: “Zonder rijst kan zelfs de beste huisvrouw geen maal bereiden”.

4. Concrete informatie over beton wordt in toenemende mate in de virtuele werkelijkheid verkregen.

5. Numerieke simulatie beoogt in de eerste plaats het vergroten van inzicht en niet het nabootsen van de natuur.

6. Een goede voorbereiding is het halve werk.

7. Succes wordt bepaald door de volharding bij het zetten van de volgende stap.

8. Beperkte kennis weerspiegelt zich in de onkunde tot vragenstellen.

9. Vele druppels vullen de zee.

10. Voor een onderzoeker is het van primair belang eerst de belangrijkste tegenstrijdigheden in een kwestie te onderkennen.

Deze stellingen worden opponeerbaar en verdedigbaar geacht en zijn als zodanig goedgekeurd door de promotor Prof.dr.ir. L.J. Sluys.

(Dutch translation by Piet Stroeven)
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