Pergamon

Cement and Concrete Research 29 (1999) 1201–1206

CEMENT AND CONCRETE RESEARCH

Assessment of packing characteristics by computer simulation

Piet Stroeven*, Martijn Stroeven

Faculty of Civil Engineering, Delft University of Technology, PO Box 5048, 2600 GA Delft, The Netherlands

Received 27 July 1998; accepted 20 January 1999

Abstract

Most relevant engineering mechanical properties of normal concretes such as compressive strength are to a large extent governed by the density and the uniformity of the aggregate packing as the load-bearing structure. Nevertheless, the integrity of this skeleton will gradually break down under increased loadings. In cementitious materials this is due to debonding of particle-matrix interfaces, which leads to crack initiation and propagation in the so-called interfacial transition zone. The strength of the interfacial transition zone on a structural level is also governed by the density and the uniformity of the packing of (blended) cement particles in the neighbourhood of aggregate surfaces. However, particularly structure-sensitive properties like cracking and tensile strength are also, and to a disproportional degree, influenced by the nonuniformity of the particle packing. This is true for microcracking that results from packing discontinuities in the binder near particle interfaces, as well as for engineering cracking at the concrete element's surfaces due to aggregate-packing discontinuities near the mould. The SPACE system (Software Package for the Assessment of Compositional Evolution) has been developed to assess the characteristics of dense random-packing situations in opaque materials by a "realistic" structural simulation. This paper presents a short introduction to the system and deals only with the essential design features. Next, an application addressing the particle-packing problems demonstrates the system's capabilities.

Keywords: Interfacial transition zone; Particle size distribution; Concrete; Modelling; Computer simulation

1. Introduction

The volume fraction of aggregate in concretes is approximately 0.65 to 0.75. Thus, packing details of the aggregate will be governed partly by deterministic and partly by stochastic influences. This is the complicated field between order and chaos, which is not easily accessible by theoretical approaches. Problems of a similar nature and complexity are found in the interfacial transition zone (ITZ), which borders particle interfaces in cementitious materials. In this case, particle sizes from the cement and eventually from fine-particle additions, which may range over two orders of magnitude, are involved. The very fine particles are added for upgrading material quality. Particularly, developments in the high strength and high performance ranges have demonstrated that these packing characteristics are of paramount importance [1–7]. In discussing very high performance concrete, de Larrard and Malier stated: "We should in fact talk about 'very-high-packing-density-concretes.' The idea behind concrete as a material is to attempt to reconstitute a solid rock from elements having complementary gradings" [6]. For that reason, analytical design tools have been developed to predict packing density, and experimental methods are in use for the same purpose.

The common approach to simulating particle packings is application of so-called "random generators," where particles of a certain range of particles sizes are sequentially positioned inside a container. Each location is randomly generated. With such high densities encountered in this category, "overlap" will occur to an increasing degree during the generation process. The solution is to reject such overlap situations, whereby the generation process is continued. Obviously, dense random packings cannot easily be generated in this way. Moreover, a more uniform structure is obtained, which underestimates natural phenomena such as clustering of particles. Therefore, a more realistic computer system for simulating particulate materials would be appropriate, particularly to study structure-sensitive properties of these materials. The system provides such tools by simulating the production process of the material (i.e., in the case of concrete: mixing of aggregates, water, and cement). The details of the generation system are published elsewhere [8]. This paper will present a short introduction to the system and will focus primarily on the major mechanisms. Then the applications to some packing problems of practical significance will be discussed.

* Corresponding author. Tel.: 0031 015 278 4035; fax: 0031 015 261 1465.

E-mail address: p.stroeven@ct.tudelft.nl (P. Stroeven)

0008-8846/99/$ – see front matter
PII: S0008-8846(99)00020-4

2. Simulation system space

The simulation approach is based on a noncontinuous representation of the internal material structure. The nonhomogeneous or granular nature of the internal material structure is represented by a set of distinct elements. Each element corresponds to a characteristic phase in the material. For example, concrete is modelled as a set of elements that represent the aggregate particles. The elements are dispersed in a presumably homogeneous mortar matrix moulded in a cuboidal or cylindrical container. The parameters that describe a static situation of the internal structure are the location, orientation, and shape of the various elements. Since the elements represent real physical phases in the material, physical properties can be assigned to each element along with their shapes and sizes, at least in principle.

The distribution of location and orientation of these nonoverlapping elements is more difficult to derive, however. To be able to simulate effects such as clustering and to reach high volume densities, element motion and interelement collision [9] are modelled, which leads to effective ingredient mixing. This stage will be referred to as the "dynamic stage."

Thus, the general simulation concept can be described as follows:

- Initially a structured or random 3-D dilute distribution of elements with predefined shape and size distribution (such as the sieve curve) is generated within the boundaries of a container. Fig. 1(a) presents the example of the starting situation of a multisized dilute mixture of spherical particles inside a cuboidal container ($V_v \approx 0.2$). Next, random linear and rotational velocity vectors are assigned to each element.
- The second step, the actual dynamic stage, is an iterative procedure where location and orientation of all elements are changed at each time step according to a Newtonian motion model. This motion model relates the element's linear and angular displacement to a set of conditions enforced on the element (e.g., gravity, friction, etc.). When elements meet during this time interval, a "contact model" defines the effect of contact on the motion/rotation update. Interparticle influences, one of the requirements for achieving a more versatile system, are obviously revealed by the contact model. This can also be realised by addition of (electrical or chemical) interparticle forces to the motion model. Higher densities are obtained by a gradual reduction in the size of the container (which compact the structure) or under the action of gravitational forces.
- Finally, the iteration stops when certain conditions are reached. Fig. 1(b) reveals such a final situation. It concerns the example of Fig. 1(a). The multisized particle system is compacted to its maximum density ($V_v \approx 0.72$, for this particular case), whereupon the resulting structure is photographically magnified for visual purposes.

The final distribution state can incorporate effects due to gravity and to interparticle influences. Relatively simple physical laws may be used to define the interparticle relationships, which introduce parameters such as mass and coefficient of friction. High densities can be obtained, which represent dense random packing states, typical for aggregate and binder particles in cementitious materials. When the container walls are considered rigid surfaces, densification leads to disturbances in the particle packing near the wall. Instead, periodic boundaries are used to simulate bulk characteristics. Wall effects are prevented in this case. Depending on macrolevel or microlevel approaches, the container wall can be conceived as the mould or as internal aggregate surfaces, respectively. For a more detailed description of the system, see Stroeven and Stroeven [8].

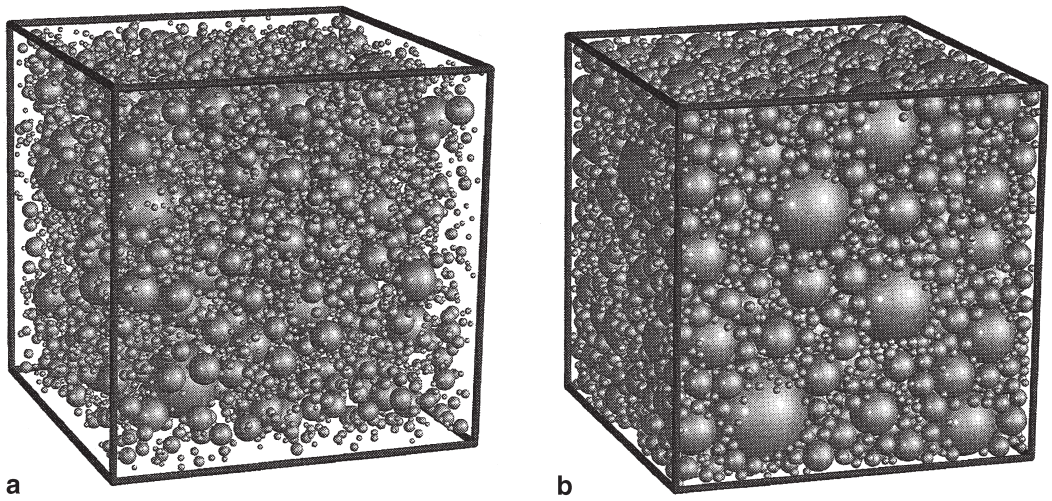

Fig. 1. SPACE system begins with a dilute system of dispersed elements. (a) Multisized spherical particles in a cuboidal container with rigid boundaries. (b) The same mixture (magnified after the process of shrinking), but compacted to maximum density.

3. Applications to particle-packing problems

The SPACE system's versatile and powerful potentialities can be illustrated by assessment of the packing structure of spherical, densely packed particles in the neighbourhood of rigid boundaries. Hence, structural discontinuities in binder particle packing in the ITZ can be studied in this way. Also, the dimensions of an outer layer of a concrete element in which the aggregate packing deviates from that in bulk can be assessed.

3.1. Particle packing near a rigid interface

For this purpose, two mixtures were generated with the container boundary assumed as rigid. The mixture of the first specimen was composed of 20% of 3-mm grains and 40% of 23-mm grains, both by volume. Hence, this can be seen as a mixture of monosized sand and gravel grains. The result is, however, not dependent on scale. So, size can also be taken to be microlevel. In that case, the mixture can be conceived as composed of monosized particle fractions of a fine mineral admixture and portland cement, respectively.

The particle size distribution of the other mixture was taken in accordance with the Rosin-Rammler cumulative particle-size distribution function (considered representative for portland cement mixtures [10]), $G(d) = 1 - \exp(-bd^n)$, with $n \sim 1$ and $b = 0.044$, and d the diameter of the particle. Particle diameters above 15 μm and below 1.5 μm were neglected. The mixture, which consisted of 15,000 elements, was compacted with rigid boundary conditions to a fractional density of 0.5 by volume (which corresponded to a water-to-cement ratio of about 0.32). Distribution of volume density of the different particle fractions in the ITZ was analysed by determination of the corresponding areal fraction in serial sections parallel to the interface.

Results on fractional volume density of the first and of the second mix are plotted in Figs. 2 and 3, respectively, as a function of the distance from the interface. Fig. 2 shows that the volume density of both grain fractions reveals an oscillatory phenomenon, which is typical for dense monosized particle systems. The relatively large number of open spaces near an interface in a monosized particle system are filled up with smaller particles in a bimodal mixture. This results in an increase in the fractional density near the interface. On another scale, such effects are encountered by blending a cement with (super) fine mineral admixtures. The patterns at the bottom of Fig. 2 represent section images parallel to the interface of the simulated particle dispersion. The picture at the left is taken close to the interface, where the density of the small particles in the mixture is highest. The picture at the right is taken at maximum density of the large particles in the mixture. Again, the finer particles are seen to concentrate close to the rigid interface.

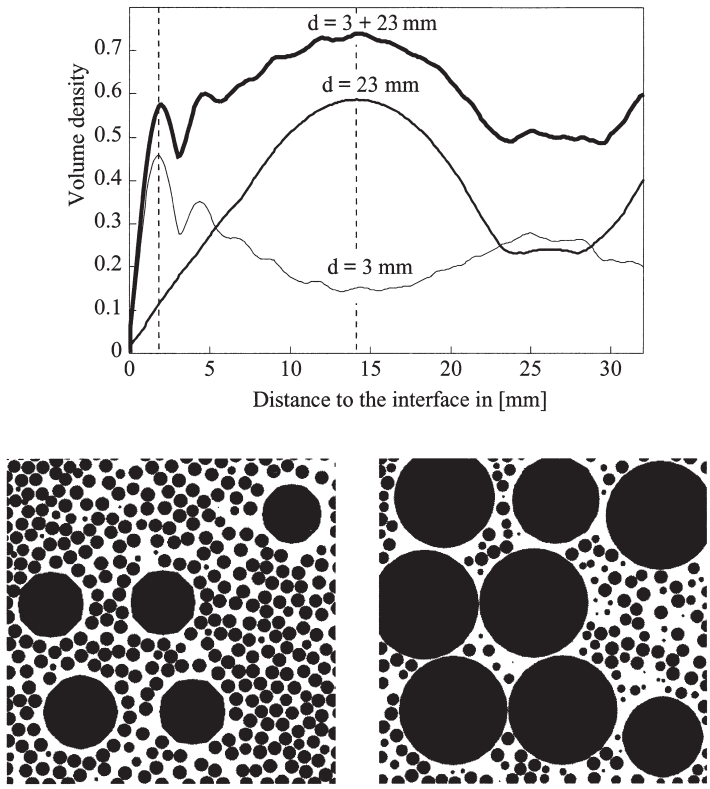

Fig. 2. Volume fraction of a bimodal particle mixture of sand and gravel is shown as a function of the distance to a rigid interface (mould). Section patterns are made parallel to the interface at distances indicated by dashed lines at the top of the figure. The partial volume density curves and the image patterns revealed boundary disturbances in particle packing that extended over a significant distance inward. As an example, compare the large differences in particle composition at ranges of 13–14 and 24–27 mm.

For the continuous-graded mixture of Fig. 3, the oscillatory effect in the overall distribution curve is no longer present. However, a significant increase in density for the smallest particles in the mixture is still obvious near the interface. Peak values in fractional volume density are approximately at average grain size distance from the interface. In contrast, in the monosized case this occurs at about half the grain size. The largest particles are obviously pushed inward by the other particles near the interface, which leads to very distinct differences in particle-size distributions in the bulk and closer to the boundary. The cumulative density curve consists approximately of three linear parts. At first a rapid increase in fractional density is observed of which the significance and extent is governed by the smallest particles in the mixture (I). The second stage (II) shows a more moderate rate of density increase. The onset of the final stage (III) coincides with the peak value of the density curve for the largest particles in the mixture. With some fine-tuning of the particle-size distribution, the angle of the slope in the second stage may be decreased, thereby seemingly decreasing the interphase depth. It can easily be seen, however, that the variation in particle composition extends over a much larger distance, and the same will hold for the discontinuity in bond strength. The conclusion is that the extent of the nonuniformity in the particle composition (which governs the thickness of the ITZ) should not be associated with the decline in overall volume density.

3.2. Optimum packing density

Optimum packing densities of a series of sand and gravel mixtures were determined in an earlier study [11]. In these experiments, a standard sand was added in various proportions to different gravel mixtures (with a particle range as in Fig. 4), whereby special attention was given to an equal-volume fraction curve and a Fuller curve. Packing density revealed optimum values for certain combinations of the sand/gravel mixtures, which was also found by Toralles-Carbonari et al. [3]. With the addition of the sand, the density of the Fuller mix increased by 10.2% (to 2.144 g/cm^3) and that of the equal volume fraction mix by 7.7% (to 2.085 g/cm^3). Overall highest density was found for an intermediate curve (E in Fig. 4).

The question could now be posed whether such problems could be approached by computer simulation as well. As a first step, the gravel structure should be reconstructed and the results should be compared with experimental data. For that purpose a series of particle mixtures were simulated by the SPACE system. Fig. 4 defines the particle mixtures A–F, in which size ranges from 1 to 32 mm. Note that this graph contains more information on the particle mixtures than a sieve curve, which is based on a very limited number of sieve-opening sizes. Curves C and F roughly correspond to the limits of the sieve curve area in the Dutch building code (NEN 2560). Of the intermediate mixes, D corresponds to the Fuller curve. These mixtures were densified by the SPACE system to their maximum density.

Of course, expectations on correspondence between outcomes of experiments and simulations cannot run too high, because of inevitable differences between both approaches. First of all, it is well known that among the various experimental methods to evaluate maximum packing density of aggregates, experimental results will vary significantly [12]. But the conditions can be varied even for one particular method, thereby additionally influencing the outcomes. In the present case, use was made of an 8-L cylindrical container in which the mixture of dry sand and gravel particles was compacted for 10 s. On the computer side, periodic boundaries were selected for correctly simulating bulk characteristics. In this way, at least the container size can be added to the factors that influenced the experimental data. In the iterative procedures of the previously described dy-

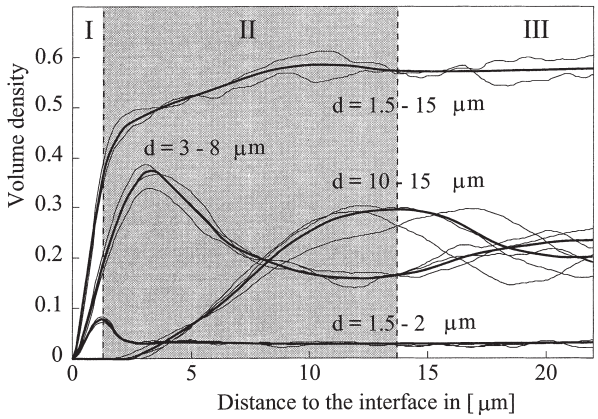

Fig. 3. Volume fraction of cement particles is shown as a function of the distance to the interface. In addition to the global (overall) value, data are presented on particle-size fractions in the mixture. Actual composition is seen to be a long-range function of the distance to the interface, a phenomenon that is not reflected by the overall curve.

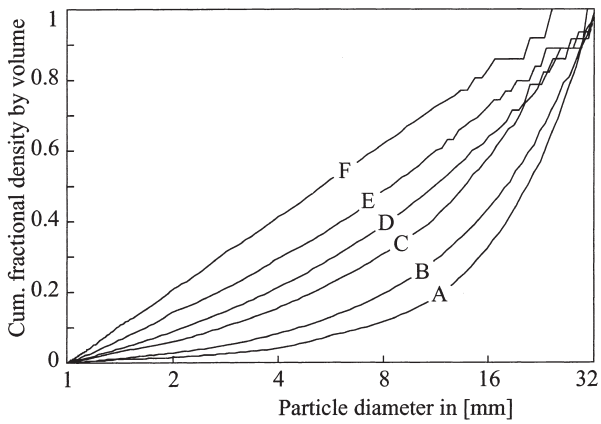

Fig. 4. Cumulative particle-size distribution function for particles between 1 and 32 mm on a semilogarithmic scale. Mixtures defined by the curves were simulated by the SPACE system.

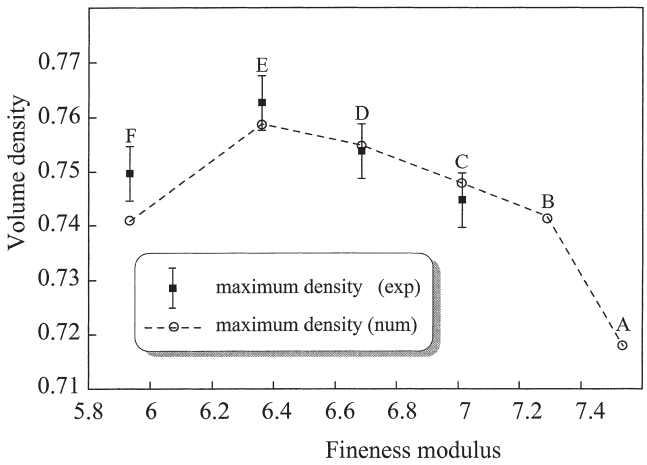

Fig. 5. Simulated and experimental values of maximum density of the mixes indicated in Fig. 4, plotted as a function of the fineness modulus; particle size ranges from 1 to 32 mm.

namic stage of the SPACE system, some particle overlap is only a temporary feature. A certain amount of residual overlap has to be accepted, however, when maximum density is approached. In the present case, the acceptance level was set at 1%, a choice that influenced the simulation outcomes. Obvious differences between the two approaches further concern the particle shape (spherical in the simulation), and the particle-size distribution curve (the underlying sieve curve of the experiments is well known to only poorly reflect the actual size distribution of the particles).

Together with the experimental data, the outcomes of the simulation are plotted in Fig. 5 as a function of the fineness modulus. Fig. 5 reveals for both approaches the highest density to be obtained for mix E, somewhere halfway between Fuller and equal volume fraction curves (on a semilogarithmic scale), which is a result of practical significance. Maximum volume density increases with declining fineness modulus from mix A to mix E. After passing this optimum, a drop occurs from mix E to mix F. In light of the foregoing conclusions, the agreement between simulated and experimental outcomes can be considered very satisfactory. These tendencies are accompanied by characteristic changes in the underlying particulate structure. As an example, Fig. 6 visualises these differences in structure by way of section images of simulated mixes B and F, which have (about) the same density (0.74).

The second step in trying to assess volume density of sand/gravel mixes by the SPACE system is to go from densified gravel (Fig. 5) to densified gravel and sand. The last problem would involve extending the particle-size range to the micrometer level. Aggregates with such a wide range of particle sizes cannot be dealt with realistically, because of the excessive number of particles involved, but the problem can be approached in a qualitative way. It is demonstrated in Fig. 6 that the Fuller curve leads to dispersed pores between the particles that are larger than those in mix F. The is due to the larger number of small particles in the latter case, which subdivide the open space into smaller pores. These smaller pores are less easily accessible by the sand without increase in overall volume. So, of the two, the Fuller curve should lead to higher densities after mixing with the sand. The SPACE can be used partly in a quantitative and partly in a qualitative sense to estimate the sand-accumulation capacity of the gravel, which leads to optimum density.

4. Conclusions

The application to packing characteristics near interfaces (either dealing with aggregate particles near the mould of concrete elements or with blended cement particles in the

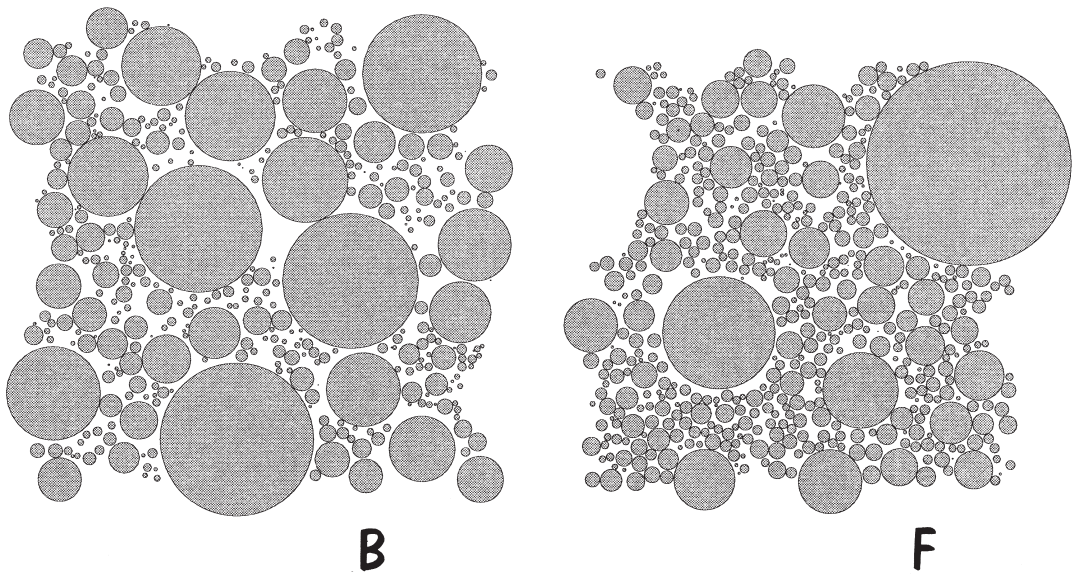

Fig. 6. Sections of the compacted particle mixtures B and F defined in Fig. 4; significant differences in details of the packing structure are visible despite an almost similar total volume density of 0.74.

ITZ) demonstrates the global density to steeply increase away from the interface and approach bulk value at a distance from the interface of the order of a particle diameter. In contrast, the discrimination to separate particle fractions in the SPACE approach shows the wave length of density fluctuations in a mixture of particle sizes to be particle-size dependent. As a result, the discontinuity in particle composition extends inward over a depth that considerably exceeds the one in global density. Since structure-sensitive properties depend on the details of particle packing, account should be given to a relatively wide interphase zone in assessment of such material properties (like tensile strength, resistance to crack initiation, and propagation). Also on the macrolevel, the discontinuity in aggregate composition will extend considerably more inward than estimated by volume density of the aggregate. This is in agreement with experimental evidence [13].

Particle-packing problems, such as dealing with the maximum attainable density of granular material of different size distributions, can be approached effectively by the SPACE system. So far, particles are assumed spherical so that shape effects are excluded.

The combination of a flexible software package combined with modern computer graphics techniques provides an excellent tool for simulating a variety of material systems. This renders possible the investigation of actual structural material properties in 3-D space. The system is versatile. By changing the element properties and interactions, in principle a wide variety of engineering materials can be studied at different levels of the microstructure. In the future, the system will be expanded to estimate mechanical or physicochemical properties by incorporation of the appropriate properties on a microlevel. For a comparison with the conventional random generator-based systems, see Stroeven & Stroeven [14].

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