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Loose and Dense Aggregate Particle Packing Models in Cement and Concrete

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Particle packing properties are important to develop high technology products in the field of cement and concrete. Two types of particle packing models for aggregates with sand and cement were introduced: the loose and the dense aggregate packing. Aggregate packing models with randomly generated sand and cement particles in the interstices of aggregates fit the Furnas model very well. Different aggregate models show different packing properties with the experimental results. Main reason for the difference with the experimental results is due to sand rearrangement in the loose aggregate packing model and to aggregate relaxation in the dense aggregate packing model. In the experimental situation, aggregates seem to be more disordered and have a relaxed packing structure in the dense packing, and sands seem to have a more rearranged packing structure in the loose packing model.

Key words: Computer, Simulation, Particle, Packing, Cement. Concrete, Aggregate

I. Introduction

Furnas[1)] introduced the idea that exact size ratio is one of the most important factors to achieve high packing density in his pioneering work. His theory of particle packing describes the ideal packing of spherical particles. Since then, many researchers have studied on the particle packing. Westman and Hugill[2)] packed particles with different sizes and showed how packing density varied for sizes having very large diameter ratios. Scott[3)] packed steel balls of equal size in two different ways, loose random packing and dense random packing. Bernal and Mason[4)] studied the difference in coordination number between the loose packing and the dense packing. McGeary[5)] used two stage packing model in order to maximize packing density, where big particles were packed first and added far smaller particles later to fill the voids among the big particles and obtained 95.1% packing density in a quaternary system. Computer simulation methods for particle packing have been extensively used after Mason[6)] assumed a central confining force and found a limiting density around 64 % for simulated monodisperse spheres. Tory *et al.*[7)] simulated the settling of spheres considering the gravity of particles. Davis and Carter[8)] introduced a Monte Carlo algorithm to simulate 3-dimensional random particle packing using a simple linear packing concept. Their algorithm was mat-ched well with the experimental results reported by Mc-Geary.[5)]

In the field of cement and concrete, Peterson[9)] used packing models in relation to the mechanical model of clinker granule during burning process in cement manufacturing kiln. Even though particle packing in cement and concrete production has been studied for a long time, main issues were rather limited to such topics as the correct type of aggregates for optimal cement and concrete properties, and the correlation between the porosity of hardened mortar and the compressive strength of cement and concrete.[10)] Pow-ders[11)] suggested that aggregate with high packing density does not necessarily guarantee the concrete having high packing density.

Optimal particle packing using cement and concrete materials has received much attention, recently, in order to develop high strength mortar and concrete. In the field of cement and concrete technology, cement and concrete proportioning is still more of an art than a science. There are still many different procedures to meet the engineering needs. The application of computer simulation technique to understand the concepts of particle packing in cement and concrete is essential to develop high technology tailored cement and concrete products. In this research, we used computer simulation technique to study, in the field of cement and concrete technology, decent cement and concrete proportioning.

II. Modeling and Simulation

One of the most important parameters in particle packing in cement and concrete is the packing density, which is the volume fraction of the system occupied by the solids. The packing density is equal to one minus the porosity of the system. Furnas model[1)] explains the ideal packing of spherical particles. Furnas model[1)] is known to be valid only in the case of diameter 1(small particle, d_1)<<diameter 2(big par-

ticle, d_2), which is typical in the field of cement and concrete. If this condition is not fulfilled, the packing density of binary mixture will depend on the diameter ratio d_1/d_2. Several other models[12] were also proposed to explain the packing behaviors observed in the packing experiments. These models consider the variations that occur in the porosity of the binary mixtures of spherical particles as a function of particle proportion.

There are two main particle packing algorithms described in the literatures in the computer simulation of particle packing. The first method[13] is to find the most stable positions available on the particle cluster surface. This method has to keep track of all outer sites available in order to pack new particles. The other method[14] is to generate particles with zero radii and to gradually increase particle radius to the target radius, where particles were moved when particles overlap each other until particles just touch. The second approach is more practical for the particle packing in cement and concrete after some minor modifications, which will be explained later in detail. In order to simulate particle packing in cement and concrete, experimental findings by Johansen and Anderson[12] were used as particle packing conditions in cement and concrete, which were summarized in Table 1. There are two types of aggregates reported. 'Aggregate Type A' shows loose packing structure and 'Aggregate Type B' shows more dense packing structure, which are similar to the packing models suggested by Scott.[3] There is huge size difference among cement, sand, and aggregate particles as shown in Table 1, which made computation necessary for the particle packing simulation in cement and concrete very difficult.

In this research, proper approximations are necessary in order to simplify computation as follows. Cement particles are assumed to be packed in the interstices of sand particles and sand particles are assumed to be packed in the interstices of aggregate particles in this simulation, which is proper for particle packing with big size ratios. The representative sizes of aggregates, 'Aggregate Type A' and 'Aggregate Type B,' are same as 14.0 mm just for simplification in computation. The size ratio of aggregate to sand is assumed to be 0.012 : 1 : 10, which will be used as a representative value. 'Aggregate Type A' and 'Aggregate Type B' are assumed to have different packing densities due to their particle size and shape during packing. Models showing similar packing densities in typical crystal arrangement are selected as aggregate packings.

Above approximations are summarized in Table 2 with

Table 1. Particle Radius Ratio and Packing Density in Packing Experiment[12]

Particle		Size (diameter, mm)	Packing Density	Size Ratio
Cement		0.017	0.50	1
Sand		1.37	0.60	80.6
Aggregate	Type A	13.6	0.49	806.0
Aggregate	Type B	14.3	0.74	838.2

Table 2. Approximations in Packing Models for Sand and Aggregates

Particle	Size, d (diameter, mm)	Packing Density, p	Model Packing
Cement	0.017	0.50	Random
Sand	1.4	0.60	Random
Aggregate Type A	14	0.52	Loose Packing (Simple Cubic)
Aggregate Type B	14	0.74	Dense Packing (Face Centered Cubic)

Table 3. Model Packings and Specifications

	Loose Packing Model	Dense Packing Model
No. of unit cell	One Simple Cubic	1/4 Face Centered Cubic
No. of particle in unit cell	1	1
Size of particle unit cell	2 r×2 r×2 r	$\sqrt{2}$ r×$\sqrt{2}$ r×2$\sqrt{2}$ r
Packing density	52 % (Simple Cubic)	74 % (Face Centered Cubic)

two kinds of aggregate model packings, simple cubic packing and face centered cubic packing, in order to simulate the loose and the dense packings in Table 1, respectively. Model packings and their specifications in Table 3 are used for packing simulation conditions in this work. The loose packing with packing density of about 52% in the loose arrangement and the dense packing with packing density of about 74.0% in the dense arrangement were used in order to simulate the loose and the dense packings of aggregates in Table 1. Eight aggregate particles were used in the loose packing and six aggregate particles were used in the dense packing, respectively.

In order to visualize the packing process, packing scale is designed on the basis of computer screen scale, which is 8× 12 in an arbitrary unit. The radii of cement, sand, and

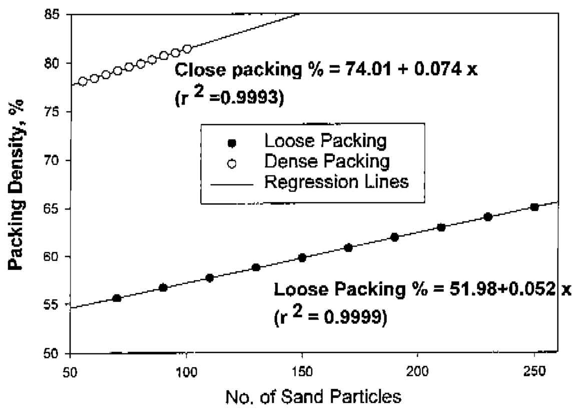

Fig. 1. Packing density of concrete calculated by Furnas model at different simulation conditions.

aggregate particles are 0.0049, 0.4, and 4.0 in screen scale, respectively. The packing densities of aggregates are controlled into 52% in the loose packing and 74% in the dense packing, which are affected by the initial arrangement of aggregate particles. Fig. 1 shows the number of sand particles used in the particle packing of concrete and the packing densities calculated by the Furnas model in case f_2(aggregate particle, f: volume fraction)>>f_1(sand particle) using following relation, where particle mixture is the matrix of small particles distributed in the interstices of larger particles.

Total Packing Density
=Packing Density/Volume Fraction of Big particle (1)

In this modeling, three stage packing is designed in order to consider big size differences, where aggregate particles are packed first and sand particles are packed later. Cement particles are assumed to be packed in the interstices of sand particles without affecting the packing structure of bigger particles. Aggregate particles are generated at the specified positions first and sand particles are generated one by one in the interstices of aggregate particles unless sand particles do not overlap other particles. When sand particles are overlapped each other, new sand particle is rejected and generated again at another random place because overlapping is not allowed in real particle packing. Fig. 2 shows the general flow chart of total packing algorithm. Sand packing process starts to run by checking the overlapping of sand particles as shown in Fig. 2. If sand particles are overlapped, the number of particle overlapping is counted in order to evaluate the speed of packing process. The maximum number of particle overlapping is fixed at ten million to avoid excessive computation time.

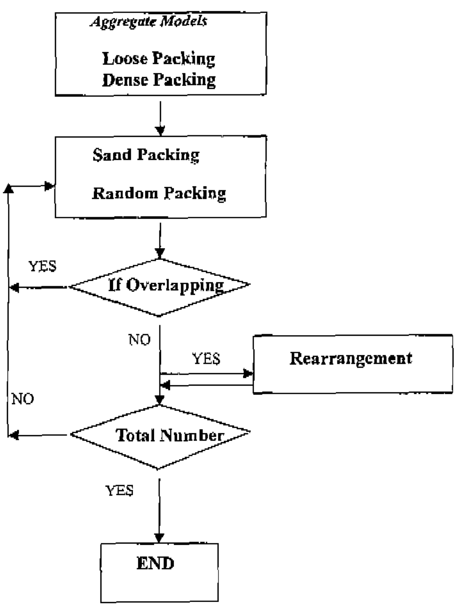

Fig. 2. Flow chart of particle packing in cement and concrete.

Table 4. Particle Proportion at Maximum Packing Density in Cement and Concrete[12]

	Loose Packing (%)	Dense Packing (%)
Cement	11	10
Sand	41	17
Aggregate	48	73
Total	100	100
Maximum Packing Density	0.78	0.82

III. Results and Discussion

As mentioned above, sand particles with equal sizes(r_1=1.4) are packed after packing aggregate particles(r_2=14). There are several important variables in ternary packing: radius ratio, relative number of particles and extent of particle rearrangement.[1,3,7,15] In the reference,[12] Johansen and Anderson reported the maximum packing density of concrete and the particle proportions at the maximum packing density of concrete as shown in Table 4. In this work, packing density by the Furnas model is calculated in the following assumption.

d_1 (small particle)<<d_2 (big particle)
d: particle diameter (2)

Two extreme cases were usually tested to verify the Furnas model.[1] In case (f_1>>f_2, f: volume fraction), the mixture is a matrix of smaller particles containing discrete larger particles. The matrix of smaller particles has a packing density p_1 and contributes to the specific volume of the mixture by f_1/p_1.

$$p=1/(f_1/p_1+f_2) \quad (3)$$

In case f_2>>f_1, the mixture is the matrix of smaller particles distributed in interstices of larger particles. Smaller particles do not contribute to the overall specific volume of binary mixture.

$$p=p_2/f_2 \quad (4)$$

The second case is closer to the experimental conditions used in this simulation. Table 5 shows the result of packing simulation, where simulated packing densities fit the packing densities by the Furnas model calculated using equation(4) very well as shown in Fig. 1. As a result, aggregate packing models used in this work simulate the Furnas model in the both packing models. When simulated data are also compared with experimental data in Table 5, aggregate and sand content is different by about 23% in the loose packing. This difference decreased a little bit with particle rearrangement to about 18%. Particle rearrangement method is to attach all the particles one another as shown in Fig. 3, where no particles are allowed to overlap in both packing and rearrangement processes. In the dense arrangement, the differences in aggregate and sand particle proportions between experimental and simulated results

Table 5. Comparisons of Particle Proportion at the Maximum Packing Density

%	Loose Packing (%)			Dense Packing (%)		
	Experimental	Simul. Without Rearr.	Simul. With Rearr.	Experimental	Simul. Without Rearr.	Simul. With Rearr.
Cement	11	11	11	10	10	10
Sand	41	17.8	22.5	17	8.1	9.0
Aggregate	48	71.2	66.5	73	81.9	81.0
Total	100	100	100	100	100	100
Maximum Packing Density	0.78	0.77	0.80	0.82	0.91	0.92

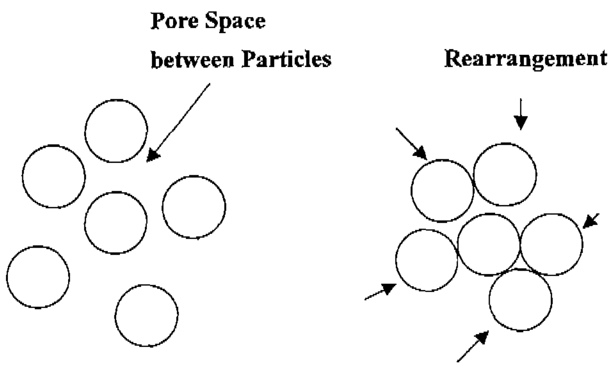

Fig. 3. Particle rearrangement process during packing.

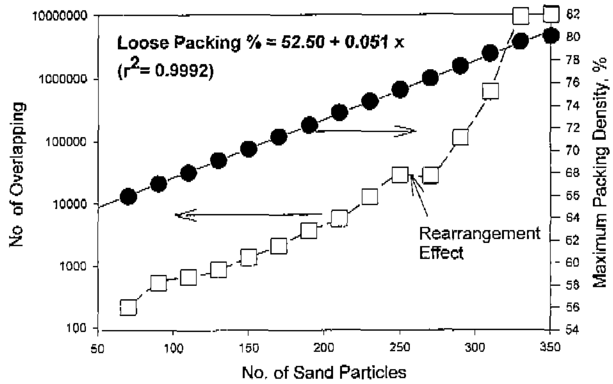

Fig. 4. Change of packing density with increasing number of small particles in the loose packing.

are only 9% without rearrangement and 8% with rearrangement. This minor difference with particle rearrangement is mainly due to the random generation of sand particles without overlapping, where sand particles can rearrange to make contacts with other particles. Simulated results in dense packing also show lower proportions in sand and higher proportions in aggregate content even after particle rearrangement.

These differences between simulated and experimental results in dense packings seem to be due to the fact that aggregate particles show more relaxed packing structure in the packing experiment due to the disorder introduced by adding sand particles in the binary packing as pointed out by Kim and Martin[15] whereas aggregates are ordered in the simulated packing. Table 5 also shows the experimental maximum packing density, simulated maximum packing density before and after rearrangement. Experimental maximum packing densities show minor differences with simulated packing densities in the loose arrangement but big differences in the dense arrangement. This big difference in the dense arrangement seems to be due to the fact that aggregate particles in the dense packing arrangement have more possibility to be more relaxed as mentioned above due to the intrinsic disorder.[15]

As a consequence, the simulated loose packing has similar packing density but big difference in the sand and aggregate proportions with the experimental results. These differences seem to be caused by the loose packing of sands particles in the simulation. The simulated dense packing has different packing density and different sand proportion with the experimental results. These differences seem to be caused by the dense packing of aggregates in the simulation.

In this simulation, maximum number of particle overlapping is limited to ten millions in one run as mentioned above. The maximum number of small particles packed in the loose packing under this limitation is around 250 before rearrangement and around 350 after rearrangement as shown in Fig. 4 and the maximum number of small particles in the dense packing is 100 before rearrangement and 120 after rearrangement as shown in Fig 5. The number of overlapping during sand particle packing increased drastically in the loose and the dense packing model, which implies computation to be more difficult drastically with

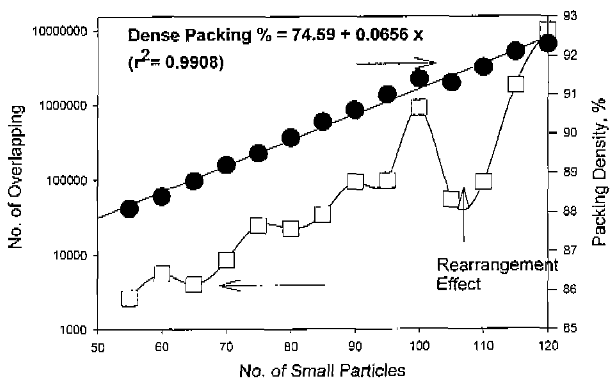

Fig. 5. Change of packing density with increasing number of small particles in the dense packing.

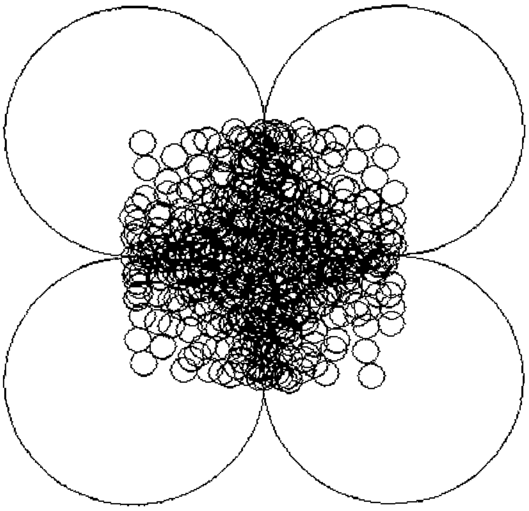

Fig. 6. Projection of particles packed in the loose aggregate packing model after rearrangement.

increasing the number of sand particles in this packing algorithm. At that time, maximum packing density is around 77% before rearrangement and 80% after rearrangement in the loose packing and around 91% before rearrangement and 92% after rearrangement in the dense packing. Fig. 6 and 7 show the projections of sand particles packed in the interstices of aggregate particles, respectively.

IV. Conclusions

Two types of aggregate packing models fit the Furnas model very well. Result on particle packing simulation in cement and concrete showed big difference in the maximum packing density with experimental results in the dense packing case but showed less difference in the loose packing case. This is due to the aggregate disordering introduced during packing experiment, where the loose packing structure receives little impact by mixing with sand particles but the dense packing structure receives much more impact by mixing with sand particles. The dense packing model does not fit the experimental result because the packing disorder in the binary packing of aggregates with sands was not considered. As a consequence, computer simulation technique is useful to predict and to explain the experimental results.

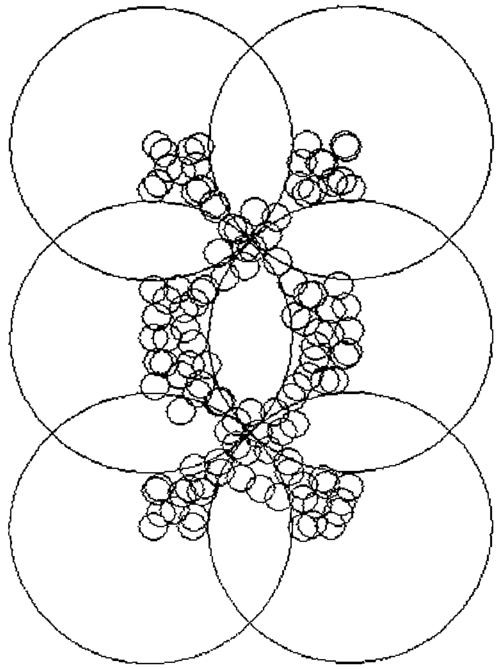

Fig. 7. Projection of particles packed in the dense aggregate packing model after rearrangement.

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