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Optimisation of aggregate gradation of ultra-high-performance concrete based on the modified compressible packing model

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The compressible packing model (CPM), which is a method for designing aggregate gradation, was used to calculate the packing density of quartz aggregate. The aggregate gradation of ultra-high-performance concrete (UHPC) was optimised using the CPM. The number of interfaces between the aggregates and cement was determined using Image-Pro Plus software. The CPM modified using the equation $Y=0.60073X+0.20551$ was found to calculate the packing density of quartz aggregate accurately. The compressive strength of the UHPC was found to be positively correlated with the packing density of the aggregate: an increase in the packing density led to a compressive strength increase from 97.9 MPa to 124.1 MPa, an increase of 26.7%. The flexural strengths of the material was found to be sensitive to the number of interfaces: the smaller the number of interfaces, the greater the flexural strength. The specimen with an interface length of 5.56 mm/mm² had the smallest flexural strength (21.5 MPa) and the specimen with an interface length of 3.596 mm/mm² had the largest flexural strength (25.9 MPa). It is recommended that, when designing aggregate gradation, a gradation with high density should be selected and the proportion of small-size aggregates should not be too large.

Notation

a_{ji}	loosening effect coefficient
b_{ji}	wall effect coefficient
d_i	particle size of i
d_j	particle size of j
$d_{\max}$	largest particle size
$d_{\min}$	smallest particle size
K	compaction index
y	volume fraction
β	virtual packing density
γ	calculated packing density
ϕ	real packing density

Introduction

Ultra-high-performance concrete (UHPC) is widely used due to its excellent mechanical properties and durability (Chen *et al.*, 2017; Xu *et al.*, 2018). Optimisation of the performance of UHPC is still a research focus in the field of concrete science (Arora *et al.*, 2019; Vincler *et al.*, 2019), in which optimisation of the aggregate gradation plays an important role. In 1999, De Larrard (1999) proposed the compressible packing model (CPM), which is a mathematical model for calculating packing density based on a large number of experiments. The model can calculate packing density with high

accuracy (Achour *et al.*, 2019; Yuan *et al.*, 2020) and is thus widely used in concrete design (Han *et al.*, 2016; Moghaddam and Baaj, 2018; Van Der Putten *et al.*, 2017).

To date, aggregate gradation theories are mainly the theoretical maximum density of the curve and particle interference theory. Fuller and Thompson (1907) proposed the theoretical maximum density of the curve, considering that aggregates with different particle sizes are combined in a certain proportion. Theoretically, aggregates have high density and low porosity. The particle interference theory, proposed by Weymouth (1933), is based on filling theory; its purpose is to obtain the maximum compactness of particles. During the long period of the development of concrete science, scientists have further optimised both theories (Bolomey, 1927; Talbot *et al.*, 1923). Shilstone (1990) and Shilstone and Shilstone (2002) proposed a coarse factor and a work factor to improve workability by controlling these two parameters. These theories all assume that aggregates are spherical particles without considering their actual shapes (Ghasemi *et al.*, 2018; Kwan *et al.*, 1999; Maerz, 2004), even though the compactness of particles of the same size but different shapes will be very different (Thirumalaiselvi *et al.*, 2018). The shape of the aggregate will clearly affect the optimal combination of aggregate but, due to the complexity of the shape factor, there is no unified theory to

Figure 1. Technical route of this study

Table 1. Calculation formulae (Bala *et al.*, 2019; Roquier, 2017)

	Formula
Particle size, d_i	$\log_{10} d_i = (\log_{10} d_{\min} + \log_{10} d_{\max})/2$
Loosening effect coefficient, a_{ji}	$a_{ji} = \sqrt{1 - \left(1 - \frac{d_i}{d_j}\right)^{1.02}}$
Wall effect coefficient, b_{ji}	$b_{ji} = 1 - \left(1 - \frac{d_i}{d_j}\right)^{1.50}$
Calculated packing density, γ	$\gamma = \gamma_2 = \frac{\beta_2}{1 - \{1 - \beta_2 + b_{21}\beta_2[1 - (1/\beta_1)]\}\gamma_1 - [1 - (a_{23}\beta_2/\beta_3)]\gamma_3}$ $\gamma = \min(\gamma_i) \quad 1 \leq i \leq 3$
Compaction index	$K = \sum_{i=1}^n K_i = \sum_{i=1}^n \frac{\gamma_i/\beta_i}{(1/\phi) - (1/\gamma_i)}$

define the shape factor of aggregates (Abyaneh *et al.*, 2013; Mora and Kwan, 2000).

In the work described in this paper, the CPM was modified, by the linear fitting method, to eliminate the influence of the shape factor on the packing density so that the accuracy of the calculation is greatly improved. The route taken in this study is illustrated in Figure 1. First, experimental and calculated values of the packing density of quartz sand were compared. The calculated values were then corrected by linear fitting. UHPC was prepared using quartz sand with different packing densities. The flexural and compressive strengths of UHPC specimens were measured to study the relationship between strength and packing density. Finally, the relationship between strength and particle size was studied using image analysis. A new method for designing aggregates for UHPC was developed.

Experimental details

The CPM

Three combinations of quartz sand particles were studied. The ternary calculation formula is shown in Table 1. The compaction index (K) of the packing density of the quartz sands was in accordance with the pouring packing process, so $K=4.1$ (Table 2). UHPC was prepared using quartz sand of three different particle sizes (1.18–0.60 mm, 0.60–0.30 mm and 0.30–0.15 mm). The measured packing densities of the three sands are listed in Table 3. Substituting these data into the formula shown in Table 1, the packing densities of the different particle size combinations were calculated.

Table 2. Values of compaction index K (De Larrard, 1999)

Packing process	K
Pouring	4.10
Vibration	4.75
Vibration + compression	9.00
Slurry	6.70

Table 3. Measured packing densities

Particle size range: mm	Packing density
1.18–0.60	0.5616
0.60–0.30	0.5352
0.30–0.15	0.4914

Raw materials

White Portland cement (P.W52.5) used in this study was provided by Jiangxi Yinshang Co., Ltd and silica fume was provided by Elkem (Shanghai) (silica content $\geq 95\%$). The quartz powder of 325 mesh and the quartz sands of 20–40 mesh and 40–70 mesh were produced in Guangxi. Polycarboxylate water reducer (SD-600P-02), with a water-reducing rate of more than 25%, was provided by Shanghai Sanrui Polymer Materials Co., Ltd.

Experimental method

The cement:silica fume:quartz sand:quartz powder ratio was 0.9:0.1:1:0.2 and the amount of water reducer used was 1.5%

Table 4. Calculated and real packing densities of different sand gradations

Sample number	Sand proportion			Packing density	
	1·18–0·60 mm	0·60–0·30 mm	0·30–0·15 mm	Calculated	Actual
1	0·35	0·40	0·25	0·5990	0·5567
2	0·35	0·45	0·20	0·5923	0·5593
3	0·30	0·50	0·20	0·5876	0·5558
4	0·30	0·55	0·15	0·5804	0·5538
5	0·30	0·60	0·10	0·5734	0·5524
6	0·25	0·65	0·10	0·5689	0·5481
7	0·20	0·70	0·10	0·5645	0·5460
8	0·10	0·80	0·10	0·5559	0·5390
9	0·55	0·10	0·35	0·6004	0·5645
10	0·45	0·25	0·30	0·5997	0·5642
11	0·40	0·40	0·20	0·5972	0·5655
12	0·50	0·15	0·35	0·5966	0·5661
13	0·70	0·05	0·25	0·6271	0·5790
14	0·50	0·30	0·20	0·6072	0·5667
15	0·50	0·20	0·30	0·6036	0·5675
16	0·60	0·30	0·10	0·6019	0·5722
17	0·80	0·10	0·10	0·6020	0·5730
18	0·15	0·25	0·60	0·5411	0·5277

of the mass of cementitious material. UHPC was prepared by changing the ratio of the three quartz sands. The dry materials were mixed for 2 min in a mortar mixer. After adding the water, the mixture was mixed for a further 8 min. Mortar specimens of size 40 × 40 × 160 mm were prepared. Tests were performed after curing the samples for a specified time.

The strengths of the specimens at 28 d were tested according to Chinese standard GB/T 17671 (CNS, 1999) and the packing densities of the specimens were tested according to Chinese standard GB/T 14684 (CNS, 2011). After crushing and polishing the samples, they were placed under a microscope, magnified five times and photographed. To count the number of aggregate interfaces, the photographs were processed using Image-Pro Plus software.

Results and discussion

Actual and calculated packing densities

Actual packing density

Eighteen different gradations of quartz sand were tested and their packing densities were determined by the CPM and testing. Table 4 shows the mass ratios of the three aggregates and the calculated and measured packing densities. As shown in the table, the calculated and real packing densities were not in complete agreement and this is because the CPM treats particles as spheres (i.e. it does not consider particle shape) (Prudêncio *et al.*, 2013). The results were fitted using the least-squares method. The fitted graph is shown in Figure 2 and the fitting equation and correlation coefficient (adjusted R^2) are shown in Table 5. The correlation coefficient between the linear fitting equation and the experimental data was determined to be 0·95276. The linear fitting equation was

Figure 2. Linear fit of the calculated packing density

Table 5. Fitting equation and correlation coefficient

Equation	Adjusted R^2
$Y = 0·60073X + 0·20551$	0·95276

thus very accurate for correcting the calculated packing density as it eliminated the error caused by the shape of the particles. Therefore, the calculated value was corrected by the equation $Y = 0·60073X + 0·20551$ for the final packing density, where X represents calculated packing density and Y represents actual packing density. Correcting the CPM with the linear fit was the key to accurate calculation of the packing density.

Packing density calculated using Matlab

After substituting the modified equation ($Y=0.60073X+0.20551$) into the CPM formula, the packing densities of all combinations of the three quartz sands were calculated using Matlab. The results are shown in Figure 3. Considering the contours in the triangle, it can be seen that the influence of the three particle sizes on the packing density was in the order $1.18-0.60\text{ mm} > 0.30-0.15\text{ mm} > 0.60-0.30\text{ mm}$. The white area in Figure 3 shows the sand combinations with the highest packing density. Particles of size $1.18-0.60\text{ mm}$ occupy the main part of the mix, with appropriate amounts of the other two particle sizes. The packing density of the quartz sand was thus optimised.

Relationship between packing density and strength

UHPC specimens were prepared using quartz sands with different gradations and their flexural and compressive strengths were measured at 28 d. The compressive strength results are shown in Figure 4 and the flexural strength results are shown in Figure 5. Comparison of Figure 4 with Figure 3 shows that the compressive strength had a good correlation with the packing density of the quartz sand: the higher the sand packing density, the higher the compressive strength of the UHPC. In particular, the areas showing high density and high compressive strength were in very good agreement. These figures also indicate that, with an increase in packing density, the compressive strength of the UHPC increased from 97.9 MPa to 124.1 MPa – an increase of 26.7%. For the samples with a compressive strength greater

than 120 MPa, the proportion of $0.60-0.30\text{ mm}$ particles was less than 10% and the proportion of particles of size $1.18-0.60\text{ mm}$ was 65–80%. Therefore, it is possible to enhance compressive strength by optimising the packing density of quartz sand, which is a new way of optimising concrete preparation.

Comparison of Figure 5 with Figure 3 shows that when the packing density of the quartz sand was higher than 0.57, the flexural strength of the sample was 23–24 MPa. However, the maximum flexural strength (the white area in Figure 5) was 25–26 MPa, which was not the area of the triangle with the highest density. The gradation of the white area was approximately 50–60% of $0.60-0.30\text{ mm}$ particles and approximately 10–13% of $0.30-0.15\text{ mm}$ particles. This result shows that there was no linear positive correlation between the packing density of the quartz sand and the flexural strength of the UHPC, but it had a certain degree of correlation with the sand gradation.

Image analysis

Three typical grading schemes of quartz sand were designed (C1, C2 and C3) and the packing densities and strengths of UHPC made with the three gradations were tested. The gradations of the quartz sand and the test data are shown in Table 6. The samples were placed under a microscope and 20 photographs of different areas were taken. Image processing software was used to grab the area of the aggregate; the photo processing process is shown in Figure 6.

Figure 3. Calculation of packing density using Matlab

Figure 4. Compressive strength results

Figure 5. Flexural strength results

The interface length (aggregate perimeter) between the cement and aggregate was then calculated using Image-Pro Plus software.

The interface lengths of the three specimens (total length of interface per square millimetre) are shown in Figure 7 and the cumulative distribution of interface lengths is shown in

Table 6. Packing densities and strengths of UHPC made with three typical sand gradations

	Sand proportion			Packing density	Compressive strength: MPa	Flexural strength: MPa
	1·18–0·6 mm	0·6–0·30 mm	0·30–0·15 mm			
C1	0·70	0·05	0·25	0·5852	124·0	23·1
C2	0·30	0·60	0·10	0·5525	106·8	25·9
C3	0·04	0·37	0·59	0·5272	98·0	21·5

Figure 6. Image analysis process

Figure 7. Interface length and flexural strength results

Figure 8. Cumulative distribution of interface lengths

Figure 8. Figure 7 shows that the packing density of the three gradations was not positively correlated with the UHPC interface length. However, it can be seen from Table 6 that the compressive strength had a good positive correlation with the packing density of the quartz sand, which was consistent with the previous results. This indicates that the compressive strength mainly depended on the sand packing density.

Comparison of the flexural strength of the three gradations with the interface length (see Figure 7) reveals that the larger

the interface length, the lower the flexural strength. The interface length of C3 was the largest (up to 5·56 mm/mm²) and its flexural strength was the lowest (21·5 MPa). C2 had the smallest interface length (3·596 mm/mm²) and the greatest flexural strength (25·9 MPa). It can thus be inferred that the flexural strength of concrete is particularly sensitive to the number of internal interfaces. This is because the larger the interface, the more weak points there are and thus the lower the flexural strength. As shown in Figure 8, the more sand particles of size 0·30–0·15 mm in the mix, the larger the slope of the curve and the greater the interface length. Therefore, when preparing UHPC, the proportion of sand

particles of size 0.30–0.15 mm should be reduced to ensure high flexural strength.

Conclusions

Based on the experimental results, the following conclusions can be drawn:

- Correcting the CPM with the equation $Y = 0.60073X + 0.20551$, which was found to calculate the packing density of quartz sand accurately, can eliminate the influence of the aggregate shape factor.
- The flexural strength of UHPC was found to be particularly sensitive to aggregate interfaces. As the number of interfaces increased, the flexural strength decreased. The specimen with the largest interface length (5.56 mm/mm²) had the lowest flexural strength (21.5 MPa) and the specimen with the smallest interface length (3.596 mm/mm²) had the highest flexural strength (25.9 MPa).
- The results of this study also showed that a higher packing density of quartz sand led to a higher UHPC compressive strength. By increasing the packing density, the compressive strength of the UHPC was increased from 97.9 MPa to 124.1 MPa – an increase of 26.7%. Thus, when designing aggregate gradations, a gradation with a high packing density should be selected and the proportion of aggregate of small particle size should be reduced.
- The use of Matlab to design aggregate gradation has many advantages, such as a small amount of tests and excellent results. It can thus be used as a new method for designing aggregate gradation.

The next step of this work will be to establish a model for particle size distribution and interface length that can accurately calculate the interface length of UHPC. Furthermore, the factors influencing strength need to be further examined. The method of designing aggregate gradations could also be extended to ordinary concrete.

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