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Aspects of size effect on discrete element modeling of concrete

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ABSTRACT

Present paper focuses on the modeling of size effect on the compressive strength of normal strength concrete with the application of discrete element method, considering specimen of different concrete mixes and shapes. An equation was derived to estimate the parallel bond strength from the compressive strength. The results showed a good agreement with the literature and the derived estimation models showed strong correlation with the measurements. The results indicated that size effect is stronger on concretes with lower strength class and that it is more significant on cube specimens than on cylinders. The relationship of model size and computational time was analyzed and a method to decrease the computational time (iterations) was proposed.

KEYWORDS

discrete element method, size effect, normal strength concrete, compressive strength, parallel bonds

1. INTRODUCTION AND LITERATURE REVIEW

Nowadays it became a well-known fact through the work of many researchers that the specimen size and shape influence the strength of concrete specimens [1–6]. Mainly because of that, the specimen sizes were standardized; the compressive strength of concrete is measured on a standard cylinder (Ø150 mm × 300 mm – 1:2 width-to-height ratio) or cube (150 × 150 × 150 mm – 1:1 width-to-height ratio) [7]. While these specimens are for compressive strength tests used, different size samples may be applied for the determination of other material properties.

The effect of size on the strength of concrete was first described in detail by Bazant [8], who derived the so-called Size Effect Law (SEL). SEL describes the dependency of strength on the size and fracture characteristics (among other factors). His work was followed by many researchers; one of the most widespread is the derivation of Kim et al. [9], which is called the Modified Size Effect Law (MSEL). MSEL is given in Eq. (1),

$$\sigma_N(d) = Bf_t^{'} \Big/ \sqrt{1 + d/\lambda_0 d_a} + \alpha f_t^{'}, \tag{1}$$

where $\sigma_N(d)$ is the size-dependent nominal strength; $f_t^{'}$ is the direct tensile strength; d is the characteristic dimension; d_a is the maximum aggregate size; and B, λ_o, and α are empirical constants. In another study, Kim et al. [9, 10] reached the conclusion that in Eq. (1) the effect of d_a can be neglected if d_a is below 25 mm. Eq. (1) gives a good estimate for cylinder specimens with higher than unique h/d ratio.

For cube strength estimation, a method was proposed by del Viso [11], which was tested on high strength concrete samples. All the above-mentioned models describe that a larger specimen (made from the same concrete mix) has lower nominal strength. Though the mechanism of compressive failure has been well investigated, the failure mechanism and its size effect have been insufficiently studied [2].

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In the literature, it was found that a possible numerical method to model the phenomena, which corresponds to the size effect of compressive strength of concrete, could be the Discrete Element Method (DEM), which allows the user to study the micro-dynamics of the material [12–14]. For the numerical verification of the laboratory test, the Particle Flow Code 3D (PFC3D) software was used, which is a powerful tool for the DEM modeling of materials.

The aggregates in the concrete are bonded to each other with cemented contacts, which can be modeled in PFC with the so-called parallel bond contact model. This type of model was initially developed for concretes and other cementitious materials. A parallel bond provides the force-displacement behavior of a finite-sized piece of cementitious material deposited between two particles. Parallel bonds can transmit both forces and moments between particles, thus parallel bonds may contribute to the resultant force and moment acting on the two bonded particles. The tuning of the model is based on the set up of the normal and shear strengths of the parallel bonds [15].

One of the advantages of DEM is that it is able to replicate the particle size distribution for a physical material; however, the computational cost of the simulations can be reduced by neglecting the finest particles. Neglecting the smallest particles is valid if it can be assumed that these particles do not play a major role in load-bearing, as it is the case of normal strength concrete, where the aggregate skeleton of coarse aggregates does the major part of the load-bearing [16]. In the present study, an analysis was performed to see the effect of the smallest element size on the main parameters of the DEM.

2. MATERIALS AND METHODS

To investigate the size effect on compressive strength of concrete, a series of laboratory experiments were conducted. As a first step, concrete mixes were designed with normal compressive strengths that are frequently applied in the industry. Therefore, five mixes of different strength classes were designed: C20/25, C30/37, C35/45, C45/55, C50/60 that cover the area of normal strength concrete. In the later sections of this study, the C20/25 concrete will be referred as Mix 1, the C30/37 as Mix 2, the C35/45 as Mix 3, the C45/55 as Mix 4, while the C50/60 as Mix 5 for easier identification. The class of the concrete was determined based on the recommendation of EN 206 standard [17]. The applied aggregate was normal quartz aggregate with 16 mm of maximum aggregate size (d_{max}) and CEM I 42.5 N Portland cement was applied. Besides the aggregates, cement, and water no other special additives were added to the mixes. The final design of the mixes and the applied component quantities can be seen in Table 1.

The applied treatment was the same for all samples.

The compressive strength of concrete was measured in the experiments on specimens with different size and shape. The shape of the sample was either cube or cylinder because these are the two standardized shapes for concrete compressive strength testing. The edge length of the cube samples was 50, 100, 150 or 200 mm, while in case of the cylinder specimens the following samples were casted (diameter $\times$ height): 60 $\times$ 120, 100 $\times$ 200 and 150 $\times$ 300 mm. These sample sizes were chosen because they are applied in the standards for different test methods. From every size and shape, three specimens were produced, which means 105 samples in sum.

Table 1. Concrete mix design

		Mix 1	Mix 2	Mix 3	Mix 4	Mix 5
Cement [kg m^{-3}]		264	380	360	500	500
Water [kg m^{-3}]		176	190	180	175	175
Aggregate [kg m^{-3}]	0/4	910	984	64	595	789
	4/8	542	358	458	425	470
	8/16	484	447	733	679	470
Fresh concrete density [kg m^{-3}]		2,377	2,362	2,375	2,377	2,403

It was aimed in this project to verify the laboratory experiments with DEM models and to see whether the size effect on compressive strength can be shown with the help of DEM or not. The applied PFC3D software uses rigid spherical elements to model the aggregates of the material (in this case concrete). The other components of concrete were modeled with contacts. The size of the elements in the model of the concrete block was based on the aggregate sizes found in the real material, so the particle size distribution of the real material was followed by setting up the parameters in *PFC3D*, according to Table 1. In case of DEM modeling, the most challenging task is the appropriate set up of the model parameters. In the present case, the compressive strength of the material was measured, for that the main influencing parameters are

- the density of the material;
- (measured) the friction coefficient between the particles;
- (0.4) the bulk modulus;
- and (3.5 GPa) the normal strength of the contacts.

The normal strength of the parallel bonds is not a real material parameter, thus it has to be set up by applying an iteration method, where this parameter is changed and the compressive strength of the material is compared with measurements. This is a typical approach in case of discrete element models. The nature of this calibration process is trial and error, carried out over iterations of simulation and parameter adjustment.

The initial parameters for the iteration process were chosen based on literature data, the recommendations of the Itasca software Development Company and previous works of the authors of this article. The above presented process leads to a two-parameter optimization problem, which can be simplified based on the work of the authors, by choosing the standard deviation to 10% [18]. When the appropriate model parameters are found, the final material can be generated and the model can be used for further investigations.

Table 2. Main results of the laboratory and numerical measurements for standard size samples

	Mix	Number of samples	Volume [m^3]	Density [$kg\,m^{-3}$]	Compressive strength [$N\,mm^{-2}$]	Parallel bond normal strength [$N\,mm^{-2}$]
Cube	1	3	0.0034024	2,328	40.19	31.50
	2	3	0.0034049	2,294	55.05	43.30
	3	3	0.0034230	2,381	57.82	45.95
	4	3	0.0033686	2,338	67.56	53.87
	5	3	0.0033857	2,336	73.62	58.50
Cylinder	1	3	0.0053938	2,377	30.01	23.00
	2	3	0.0053325	2,317	48.83	38.50
	3	3	0.0052429	2,426	51.53	40.65
	4	3	0.0054897	2,312	61.11	48.20
	5	3	0.0054692	2,334	66.74	52.50

The parametrization of the model was carried out for every mix as well as for every size and shape. It is a time-consuming process and it increases with the dimensions of the model. Therefore, improving the performance of the simulations helps speed up the process [19], developing a simplified calibration methodology can have a great impact on future studies [20]. This indicates that, if a proper correlation between the model parameters and the size of the sample can be found, then the computational time can be decreased heavily. The parameter set up can be performed on a smaller model and then with an expression calculate the necessary model parameters for a larger model. To cancel out the effect of random arrangement of particles 5 models were created for every mix, size, and shape, as it is advised by Potyondy and Cundall [21]. All the five models had the same parameters only their particle arrangement was different. In the results section, the average of those five models is presented. Thus only for the size effect analysis, 5(mix) $\times$ 7(size&shape) $\times$ 5(particle arrangement) = 175 models were created.

To optimize the parameters (S, B, α) in Eq. (2), the nonlinear adaptation (Levenberg-Marquardt) of least squares method with a Sum of Squared Errors (SSE) cost function was applied. This method was chosen based on prior investigations.

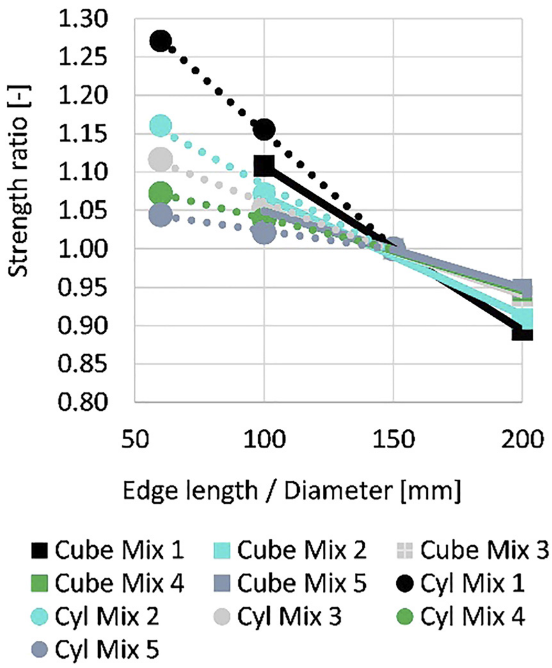


Fig. 1. Strength ratio (compared to standard size specimens) vs. edge length/diameter for all mixes (cube and cylinder results separately)

3. RESULTS AND DISCUSSION

The laboratory test results showed good agreement with the literature data with the increase of the size of the samples the compressive strength shows a decreasing trend on both cube and cylinder samples [1–7].

As an example, Table 2 contains the main results of the standard size samples' (150 mm edge length or diameter) laboratory and numerical measurements.

If the measured compressive strengths of all samples are compared to the standard strength then it gives the strength ratio plotted in Fig. 1. An interesting observation can be done based on the figure: among different mixes, with the decrease of the compressive strength the specimen size has an increasing effect. It can be seen that the differences in strength ratios are much higher in case of Mix 1 than in case of Mix 5. This means that in case of concretes with lower compressive strength the specimen size has an even more important role. It can be explained by the more extent heterogeneity of the material. Moving towards the higher strength concretes the material becomes more and more homogeneous and thus the number of potential internal structural errors decreases.

3.1. Size effect law of parallel bond strength

Equation (1) can be generalized to contain only one size dependent variable (d), which may be applicable for both cubes and cylinders. And as it was discussed earlier in DEM models the parameter that has the highest effect on the compressive strength result is the parallel bond normal strength. Thus a modified version of MSEL applicable for parallel bond normal strength could be proposed. It could be written in the following form:

$$\sigma_{pb}(d) = Bf'_{pb} \Big/ \sqrt{1 + d/S} + \alpha f'_{pb}. \quad (2)$$

Based on this model (if the specimen size and the standard compressive strength of the sample are known), the nominal parallel bond strength of the given sized sample can be determined.

Based on the parallel bond strength results of the numerical experiments (see Table 2), model equations have been defined for all mixes (for cylinders and cubes as well) to estimate the parallel bond strength based on the volume of the sample. The model equations were applied as an interpolation to calculate the expected parallel bond strengths for given volumes. The chosen range of volume was divided uniformly into 8 points in which the parallel bond strength was determined. In this way the number of measurements has been enriched, which could be used for the verification and validation of the proposed model, leading to a presumably more accurate approximation. The smallest value of 0.0002 m^3 was chosen to be about the same as the smallest specimen (this can be considered as an elementary unit; the smallest size where 3 of the d_{max} size aggregates fit next to each other), while the maximum value was chosen to be the same as the size of the largest specimen.

The parameters in Eq. (2) were tuned, using the so obtained data as the measured output of the optimization scheme. One of the aims of the research was to apply Eq. (2) with different optimized parameter sets to estimate the parallel bond strength of different size specimens.

The initial conditions were chosen to be the same for all the parameter tuning (the values defined by Kim and Eo [9] for compressive strength). B was chosen to 0.4 [-], α to 0.8 [-] and S to 50 mm. Then the optimization process was performed (least squares method; SSE objective function). The optimized parameters for the different specimen shapes can be seen in Table 3.

In most practical cases the parallel bond strength of a standard size specimen is not known, but rather the compressive strength of the standard size cylinder/cube. So the relationship of the parallel bond strength and compressive strength of standard size specimens was investigated. It was found that the same linear relation can be written for both cylinder and cube specimens, as it can be seen in Eq. (3) and Fig. 2,

$$f'_{pb} = 0.79 f'_c. \quad (3)$$

The results of the estimation process were evaluated on the basis of $\sigma_{pb}(d)/f'_{pb}$ as the function of the volume. In Fig. 3, the results for estimating cylinder strength are shown from the measurements (Mix 1–5) and from the own estimation model. The results show that with the increase of the specimen size, the strength ratio approaches a limit. It can be read from Fig. 3 that the estimation model (Cyl-to-Cyl the cylinder specimen strength calculated from standard size cylinder specimen) strongly correlates to the measurement results, especially in case of larger size specimens. In this evaluation methodology, the Cube-to-Cyl estimation models

Table 3. Optimized parameters based on specimen volume

Shape	B [-]	α [-]	S [mm]
Cylinder	1.967	0.09	40.698
Cube	1.614	0.101	66.767

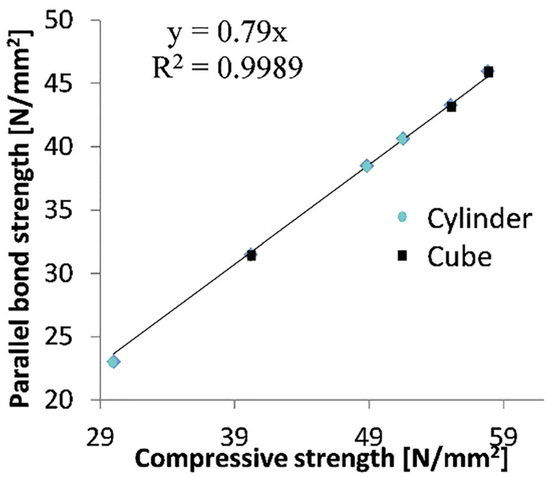
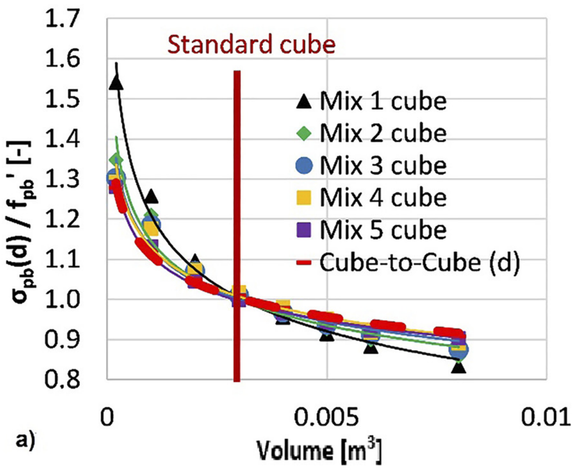


Fig. 2. Parallel bond strength vs. compressive strength for standard size specimens



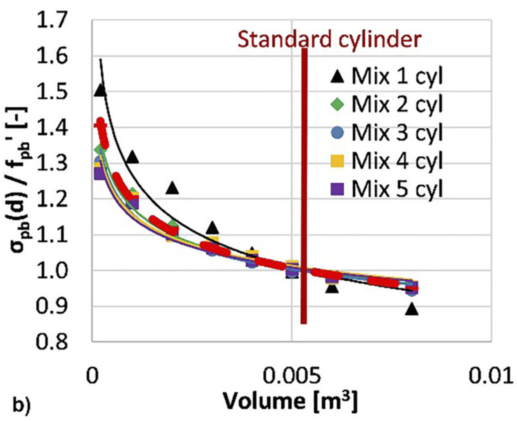


Fig. 3. Results for estimating a) cube and b) cylinder strength (dashed – own models; solid – measurements)

coincide with the Cyl-to-Cyl models (they apply the same parameter set, only f'_{pb} is different).

The Cube-to-Cube estimations also show good correlation with the measurement data, similarly to cylinders, as it can be seen in Fig. 3. The correctness of the models is shown in Fig. 3, the $\sigma_{pb}(d)/f'_{pb}$ ratio is equal to 1 for all models and measurements at the volume of the standard size specimen. Figure 3 shows that the size effect is more significant in case of models with lower standard parallel bond strength, similarly to compressive strength as it was mentioned earlier (Fig. 1). The maximum and minimum values in case of Mix 1 (which has the lowest strength class: C20/25) are 1.54/1.50 and 0.83/0.89 for cubes/cylinders respectively, while in case of Mix 5 (which has the highest strength class: C50/60) these values are 1.28/1.27 and 0.90/0.95. The deviation of the values in case of the higher strength class specimen is significantly lower, as it is shown in Fig. 3. The dependency on size can be traced back to the size dependence of compressive strength on concrete specimens. As it was mentioned earlier in this section, it is caused by the level of inhomogeneity of the different mixes. In case of a lower strength concrete, the difference in compressive strength and Young's modulus between the cement matrix and the aggregate is significant, while in case of higher strength, the difference is decreasing. It is also worth mentioning that a lower strength concrete can be produced by many different mixes (different *v/c*, *h/c*, compacting, etc.), while in case of a higher strength concrete, there are not that many variations. From the figures it can be also read that size effect is more significant on cube samples than on cylinder samples. When the difference in $\sigma_{pb}(d)/f'_{pb}$ for the largest (0.008 m^3) and smallest specimen (0.0002 m^3) is taken in case of cubes (Mix 1: 0.71; Mix 2: 0.49; Mix 3: 0.43; Mix 4: 0:40; Mix 5: 0.38) the values are always higher than the values in case of cylinders (Mix 1: 0.61; Mix 2: 0.39; Mix 3: 0.36; Mix 4: 0.33; Mix 5: 0.32). In case of a 1:2 ratio cylinder during compressive strength test, the middle 1:1 ratio zone becomes purely compressed (without tension), while in case of a cube, there is no such zone. Therefore, only a fraction of the whole volume of the cube specimen is taking part in the load bearing, thus all small failures have a higher effect on the compressive strength.

3.2. Error analysis

Error analysis was performed to see how accurate the different estimation models are. The parallel bond strength was estimated and compared to the measurement data by using the previously obtained optimized parameter sets. The error in N mm^{-2} and in % (based on the standard cylinder/cube parallel bond strength) was calculated for every size, for every estimation model, and for every mix (Fig. 4). In the figure, both the average and the maximum errors are plotted. The first reflects the accuracy of the model, the second shows its robustness (how accurate it is for very different concrete mixes). Low average error (2.8%) and maximum error (13.5%) were performed by the Cyl-to-Cyl model. The Cube-to-Cube model performed somewhat worse in this aspect. The average error of Cube-to-Cube model can be considered as low, but their maximum error is significant. It is interesting to point out that in average error, there was relatively small difference between the two models; however, in case of maximum error, the difference is more significant (16.1%). This analysis reflects that the estimation of cylinder parallel bond strength always shows lower average and maximum error, than the estimation of cube parallel bond strength using these models.

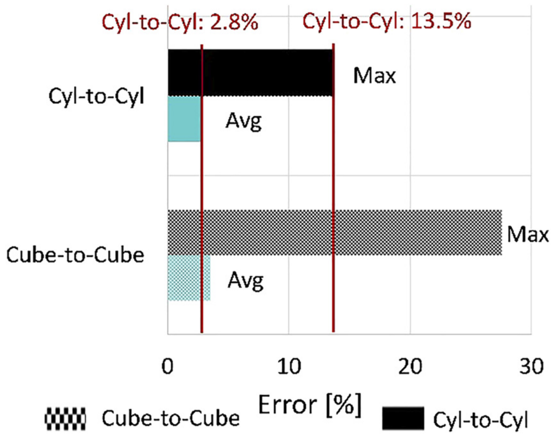


Fig. 4. Average and maximum error of the different estimation models

It was also investigated that till which size can the model be considered as sufficiently accurate. The aim here is to find the smallest specimen size that can be applied for parameter tuning of a DEM model. In Fig. 5 the average error of all models and their standard deviation is shown on the left, while on the right side the separate models' error is shown versus the specimen size. It can be clearly seen that the best fit is somewhere in the middle of the presented range, which size belongs to a 140–160 mm edge length cube or 120–140 mm diameter cylinder. A limit value was defined based

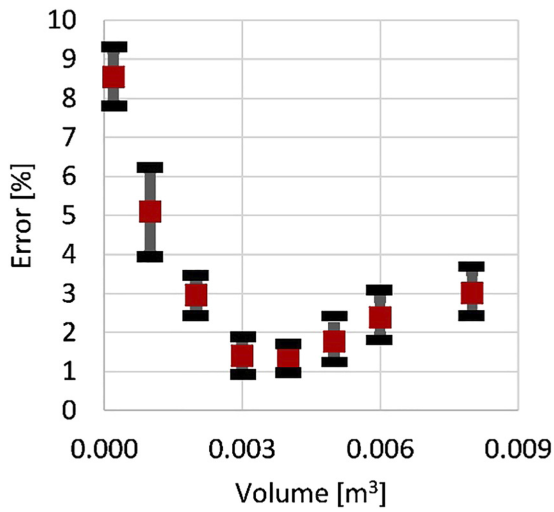


Fig. 5. Average error of all estimation models and their standard deviation

on the compressive strength classes of concrete. The model is considered to be accurate until due to the error the investigated concrete's strength class does not change. In the range of normal strength concrete, the smallest difference (in %) between two strength classes are between the C45/55 and C50/60, which is 5%. According to Fig. 5, the error and its standard deviation become too high around 0.001 m^3 (~100 mm cube or 86 mm cylinder). Thus, it is recommended to use at least a 120 mm cube or 100 mm cylinder to the parameter tuning of a discrete element model. However, using a specimen with this size makes it possible to tune the parameters even for a 200 mm edge length cube or 170 mm diameter cylinder with acceptable precision. With this significant amount of computational time can be spared. As an example, an iteration of the material genesis process of a 170 mm diameter cylinder takes around 22–24 h, while for the 100 mm diameter cylinder it is only 5–7 h.

4. CONCLUSIONS

The main findings of the research are the following:

- A linear equation was defined to estimate the parallel bond strength of a standard size specimen from the compressive strength of a standard size specimen measured in laboratory, independently of its shape (either cube or cylinder);
- Both the Cyl-to-Cyl and Cube-to-Cube model results showed good correlation with measurement data, however, the Cube-to-Cube model has higher maximum error;
- It was found that size effect is more significant for concretes with lower strength class (e.g., C20/25) due to the higher level of inhomogeneity of the material. This observation can be made with a different process only considering the laboratory measurement results as well. This observation is also true in case of parallel bonds as well. The size effect on parallel bond strength is more significant in case of lower standard parallel bond strength;
- It was also investigated that which is the smallest size for which the model can be considered as sufficiently accurate to use for parameter tuning and material generation of DEM models. It was found that using a 120 mm cube or 100 mm cylinder the compressive or parallel bond strength of a 200 mm edge length cube or 170 mm diameter cylinder can be estimated with acceptable precision. This leads to a significant reduction in computational time.

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