The influence of “up-scaling” on the results of particle method calculations of non-cohesive soils

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ABSTRACT: From a theoretical point of view particle or discrete element methods should be more suitable for the modeling of the behaviour of non-cohesive soils like sand or gravel than approaches based on the continuum theory. But, for a practical calculation it is necessary to “up-scale” the grain diameters of the soil. In this paper the effect of the scaling factor on the results of calculations with the particle method is investigated and analyzed. Triaxial tests of sand with a given grain size distribution are modeled using different scaling factors. The model parameters are calibrated by comparing the numerical results with experimental results. Additionally, an oedometer test is being modeled using the calibrated parameters for the different scaling factors. The results show that a remarkable scale effect exists. Thus, the parameters of the model have to be adapted by means of a new calibration procedure if the scaling factor is changed.

1 DISCRETE ELEMENT METHOD

Discrete element methods are being increasingly used to simulate the mechanical behaviour of granular materials (Cundall & Strack 1979, Corkum 1986, van Baars 1996, Ni et al. 2000, Thornton 2000, McDowell & Harireche 2002). In the DEM the interaction between particles is regarded as a dynamic process achieving a static equilibrium when the internal forces are balanced. The dynamic behavior is represented numerically by a time stepping algorithm using explicit time difference scheme.

This procedure of DEM takes advantage of the idea that the duration of the time step is selected and defined in a certain way that, during a single time step, disturbances in the state of equilibrium can spread only from the regarded particle to its direct neighbours. Each calculation cycle includes two stages: the application of simple interaction law at particle/particle or particle/wall contacts involving contact forces and relative displacements; and the application of Newton’s Second Law of motion to determine the particle motion resulting from any unbalanced forces.

Each contact force has a normal and a tangential component calculated from the numerical overlapping of the particles using normal and tangential stiffness coefficients. A Coulomb type friction coefficient between particles limits the tangential contact forces. A similar behaviour is adopted for the particle/wall contact.

The DEM program used in this study is PFC^{3D} (Itasca 1995). The model used in PFC^{3D} can be regarded as a sub-class of the distinct element method since it allows finite displacements and rotations of discrete bodies including detachment. It also recognizes new contacts automatically as the calculation progresses.

The program used has the following characteristics:

1 The particles are considered as homogeneous rigid balls.
2 The interaction between them is described as a soft contact, which occurs over an infinite small area.
3 The particles are allowed to overlap slightly at the contact points.
4 The slip condition between particles is governed by Mohr-Coulomb friction.

For the purpose of this study two more constraints are also applied:

1 The magnitude of the overlap is linearly related to the contact forces.
2 No tensile forces between particles are allowed.

2 MODELING OF TRIAXIAL TESTS

2.1 *The material used*

For calibration, the numerical modeling has been performed simulating Karlsruhe medium sand to compare the numerical results with experimental ones. Karlsruhe sand consists mainly of subround quartz grains. The grain size distribution of this material is given in Figure 1. The index properties of the sand are given in Table 1. The behaviour of Karlsruhe sand in triaxial tests was investigated by Kolymbas & Wu (1990). Results with dense samples (e_0 = 0.53) for different confining pressures (σ_3) are shown in Figure 2.

Table 1. Index properties of Karlsruhe medium sand (Wu & Kolymbas 1991).

Unit weight of the grains, kN/m^3	26.5
D_{10}, mm	0.240
D_{60}, mm	0.443
Uniformity coefficient, C_u	1.85
Min. void ratio, e_{min}	0.53
Max. void ratio, e_{max}	0.84

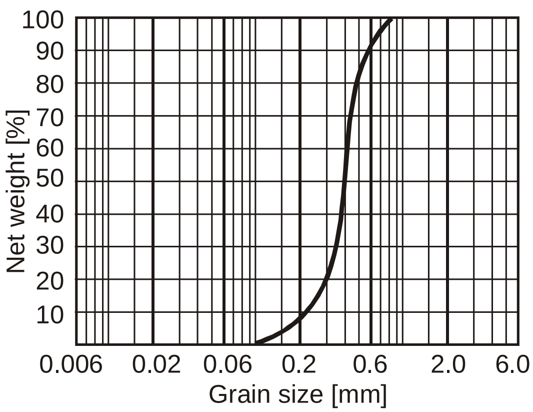

Figure 1. Grain size distribution curve of Karlsruhe medium sand (Wu & Kolymbas 1991).

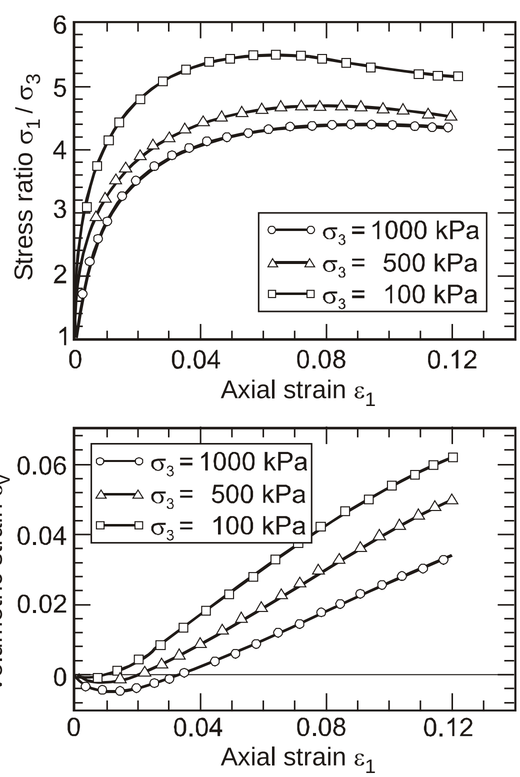

Figure 2. Experimental triaxial test results for dense Karlsruhe medium sand (Kolymbas & Wu 1990).

It is evident from the experimental results that the stress-strain-behaviour of sand is highly non-linear. A purpose of the experimental study was to investigate the effect of the pressure level on the mobilized friction angle. The results indicate that the mobilized friction angle (ϕ) - represented as stress ratio - decreases as confining pressure increases. Additionally, the dilatancy is suppressed by increasing the confining pressure.

2.2 *The geometrical model*

For the numerical model, from practical point of view it is necessary to up-scale the grain diameter of the granular soil. Such a scaling process means the horizontal translation of the grain size distribution of Karlsruhe sand. This leads to a smaller number of grains to enhance the computer efficiency to model the problem. In order to study the effect of up-scaling three different up-scaling factors have been used: usc = 20, usc = 25 and usc = 30.

The dimensions of the model were chosen according to the German code DIN 18137, which implies that the dimensions of the test sample should be greater than ten times the biggest grain diameter. Using three different up-scaling factors, the dimensions should be calculated using the largest factor of usc = 30. In order to obey this rule, the dimensions of the model were chosen to be 25 × 25 × 25 cm. The number of particles required to fill the geometrical model for different up-scaling factors are shown in Table 2.

Table 2. Number of particles for different up-scaling factors.

Grain diameter intervals [mm]	Up-scaling factors 30	25	20
0.10 – 0.20	2959	5113	9988
0.20 – 0.40	2379	4111	8030
0.40 – 0.60	399	690	1348
0.60 – 0.90	45	78	150
Σ	5782	9992	19516

2.3 *Modeling procedure*

The sample of synthetic material in *PFC^{3D}* is represented as an assembly of spherical particles. The triaxial test was modeled by confining a cubic sample within six walls. The top and the bottom walls simulate loading platens and the lateral ones simulate the confining pressure experienced by the sample sides. The sample is loaded in a strain-controlled fashion by specifying the velocities of the top and the bottom walls. Ideal test conditions were simulated by setting the friction coefficient between the sample and the walls to zero, thus avoiding any friction between the sample and the loading platens.

During all the stages of the test, the velocities of the lateral walls are controlled automatically by a numerical servo-mechanism (Itasca 1995) that maintains a constant confining stress within the sample.

2.4 *Sequence of analysis and modeling results*

During the calibration process the model parameters (normal stiffness k_n, tangential stiffness k_s and friction coefficient μ) were determined by comparing the experimental results with the numerical ones. The normal contact stiffness was chosen to $k_n = 2\ 10^7$ N/m in order to match the results and to ensure that the overlaps between the particles are very small compared to the grain diameters.

The stress-strain-behaviour of the sample for small strains (i. e. in the elastic region) is mainly influenced by the ratio of shear contact stiffness to the normal one. This ratio determines the Poisson ratio of the material. For the up-scaling factors usc = 25 and usc = 30 a ratio of 1.0 was found to match best with the experimental results.

The peak stress ratio is dependent on the friction coefficient chosen. The higher the μ chosen, the higher the calculated peak stress. Best results were achieved with $\mu = 10$, a further increase did not yield a better agreement with the experimental results.

The numerical results obtained with the parameters reported in Table 3 for a confining pressure of $\sigma_3 = 100$ kN/m^2 are shown in Figure 3.

Table 3. Microscopic parameters of the particle model.

Normal stiffness k_n (N/m)	2×10^7
Tangential stiffness k_s (N/m)	2×10^7
Friction coefficient μ	10

The results indicate that the non-linear stress-strain-behaviour of sand including dilatancy is covered by the numerical model. However, even with the chosen high value of $\mu = 10$ the peak stress ratio found in the experimental test is not reached. Obviously, the effect of the particle shape (angularity of the real grains) can not be matched perfectly by increasing the friction coefficient for spherical particles.

An important result is that there exists a remarkable scale effect, especially between usc = 20 and the other two factors (usc = 30 and usc = 25). This means that in general for different up-scaling factors different calibrated parameters should be used. For usc = 20 a better agreement with the experimental curve was found for a smaller tangential stiffness k_s.

Additional calculations were carried out to investigate if the stress level effect reported by Kolymbas & Wu (1990) is covered by the numerical model.

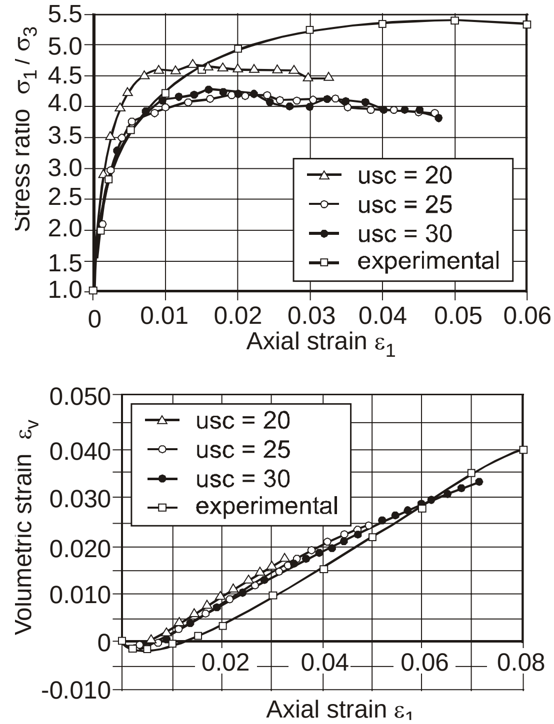

Figure 3. Stress ratio and volumetric strain plotted against axial strain for dense Karlsruhe medium sand (σ_3=100kPa)

Figure 4 gives numerical results for confining pressures of $\sigma_3 = 100$ kN/m^2 and $\sigma_3 = 1000$ kN/m^2 obtained with usc = 25. A qualitatively good agreement with the experimental results is found. Both the decrease of the stress level and the suppression of dilatancy with increasing confining pressure are obtained with the calculations.

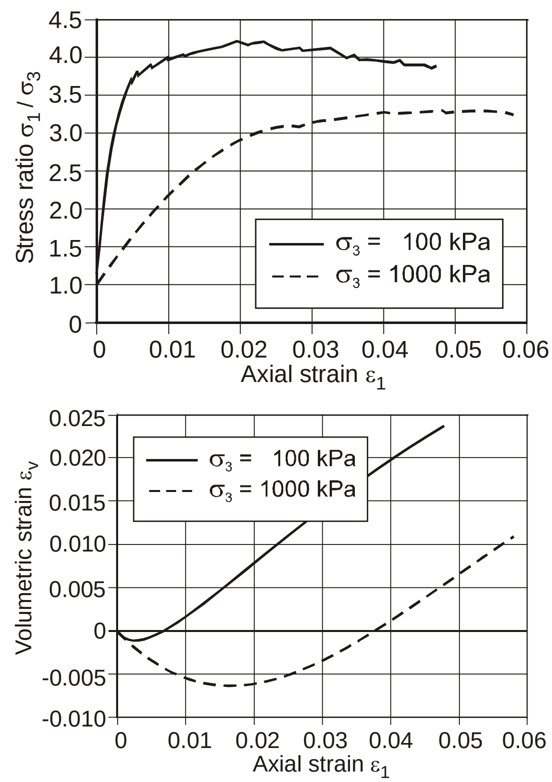

Figure 4. Numerical triaxial test results for different confining pressures (usc = 25).

3 MODELING OF OEDOMETER TESTS

A standard oedometer test consists of a circular metal ring containing a cylindrical soil sample. The sample is loaded only in the vertical direction, via a top platen, by applying increments of load until a desired stress level is reached. After each load increment is applied sufficient time is usually allowed for full dissipation of any excess pore water pressure. Results from oedometer tests are normally presented in a void ratio-axial effective stress diagram.

After modeling the triaxial test using Karlsruhe sand and calibrating the input parameters, an oedometer test as a second element test was modeled and calculated using the calibrated parameters obtained from the triaxial test. The same up-scaling factors (usc = 20, usc = 25, usc = 30) were used for modeling this element test.

3.1 *The geometrical model*

The dimensions of the model should be chosen according to the German code DIN 18135, which implies that the sample height should be at least ten times the biggest grain diameter.

Using three different up-scaling factors, the dimensions should be calculated using usc = 30. Following the above-mentioned rules, the dimensions of the model were chosen to be 25 × 25 × 25 cm. Thus, the same dimensions as for the triaxial test simulation were used.

3.2 *Modeling procedure*

The modeled particles were placed in a rectangular sample (25 × 25 × 25 cm) within six walls as shown in Figure 5. The top and the bottom walls simulate loading platens and the lateral ones simulate the confining ring surrounding the sample. The sample is being loaded in the vertical direction by specifying the velocities of the top and the bottom walls, while the side walls are kept fixed during the test. The sample was then unloaded by raising the top wall and lowering the bottom wall at the same velocity as used during initial compression, and then reloaded at the same rate past the point of maximum vertical stress achieved in the virgin compression.

3.3 *Modeling results*

After the sample had been generated, the numerical test was carried out by moving the upper and lower platen in the vertical direction and the sample was allowed to come into equilibrium. A constant vertical velocity was then applied until an axial strain of 4.0 % was reached. Figure 6 shows the results of the load-unload-reload compression sequence for up-scaling factors of usc = 20 and usc = 25. The void ratio measured at the center of the sample is plotted against the logarithm of vertical stress, calculated from the forces acting on the external walls.

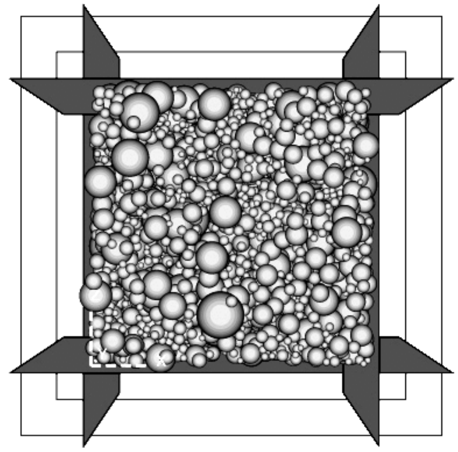

Figure 5. Numerical model for oedometer test (Top view, usc = 30, initial state).

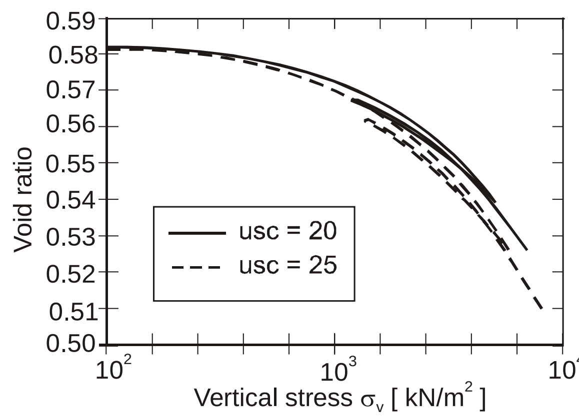

Figure 6. Numerical results for oedometer test with up-scaling factors usc = 20 and usc = 25.

It can again be stated that qualitatively there is a good agreement between the numerical results and experimental behaviour of sand. From the calculated curve, a stiffness modulus $E_s = \Delta\sigma_v/\Delta\varepsilon$ of 120 MN/m^2 was determined for a vertical stress increase from 500 to 1000 kN/m^2. This value matches those gained from experience. This indicates that the parameters calibrated by comparison with triaxial test results can be used for problems with different boundary conditions.

However, the numerical results show again a remarkable scale effect. Using the same parameters, a "weaker" behaviour of the numerical model with the larger up-scaling factor is found. This confirms the result obtained in the modeling of the triaxial tests, that in general for different up-scaling factors different calibrated parameters should be used.

An interesting result is also that the numerical results show relatively high swelling response by unloading compared with experimental results of real sand. This effect was also reported from Corkum (1986).

4 CONCLUSIONS

Numerical modeling with the *PFC*^{3D} program of two different element tests (triaxial and oedometer tests) have been carried out to investigate the effects of up-scaling on results of discrete element modeling for sand. First, three different up-scaling factors have been used for modeling triaxial test and the model parameters were determined by comparing the numerical results with the experimental ones. Then a second element test (oedometer test) was performed using the calibrated parameters.

The main conclusions are as follows:

1 Concerning a qualitative aspect, the highly non-linear behaviour of sand in both element tests is covered by the numerical model. However, the numerical model underestimates peak stresses. This is probably due to the idealization of the angular grains by spherical particles in the model used.

2 The up-scaling factor influences the results of the numerical model. This means that in general a new calibration procedure should be carried out when the up-scaling factor is changed. In the numerical tests it was found that, keeping the other parameters constant, a sample reacts weaker when the up-scaling factor is increased.

3 The calibrated parameters obtained from the first element test (triaxial test) could be used to simulate another element test, taking into consideration the effect of particle size.

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