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EFFECT OF PARTICLE-SIZE-SCALING ON PARTICLE INTERACTIONS IN DEM-SIMULATIONS OF SAND IN THE CONTEXT OF AIR PLUVIATION

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Abstract. DEM (discrete element method) is a widely used numerical simulation method, which models the behaviour of a bulk substrate based on the individual interactions of many particles. One of its possible applications is the modelling of sand behaviour in different laboratory tests, e.g., cone penetration tests [1] or direct shear tests [2]. Furthermore, DEM is specifically of interest as a modelling method for investigating air pluviation, because it models the individual inter-particle and particle-environment interactions, both friction and collisions, which determine the compaction and homogeneity of the created samples.

However, one disadvantage of DEM is the relatively long computational time [3] especially with decreasing particle sizes. This makes larger particle sizes compared to reality more interesting, especially for large scale or repeating simulations. On the other hand, if the size of the chosen particles is too large, certain interactions, such as interactions with other materials and equipment, may not be simulated in a way that properly represents real behaviour. This would lead to preferring smaller sized particles, which again would lead to longer computational times.

Therefore, the chosen particle size as an important aspect of DEM simulations will be discussed, as well as the effects on different simulation aspects. This includes necessary parameter calibrations, the resulting inter-particle and particle-environment interactions as well as the achieved simulation results and accuracies. Of specific interest is the largest particle size, at which accurate and realistic results concerning real-world particle interactions can be achieved. Further, the effects of graded particle sizes to better represent the sand during the pluviation process will be discussed.

1 INTRODUCTION

Air pluviation is a method in geotechnics for creating reconstituted sand samples for laboratory experiments or physical modelling tests. It has shown to be able to create a wide range of densities while the sample remains homogenous, even in large-scale samples [4]. However, several aspects of the pluviation process, such as interactions with mechanical parts of the set-up, influences on possible grain size separation and achieved particle size distribution have not been fully investigated. Here, numerical simulations could give insights into the particle-particle and particle-environment interactions, which influence these processes. One possible method for the numerical simulation is the discrete element method. Due to its ability to portray the interactions between individual particles [3], it is suitable to investigate the above-described aspects.

However, DEM simulations have one major disadvantage. The computational time necessary for the numerical simulation is large [3], especially with decreasing particle size and increasing particle numbers. Therefore, it is not feasible to use real world grain sizes for most simulations. Sand particles used in pluviation can be smaller than 0,2 mm and even small-scall simulations could require millions of particles at this size. Therefore, increasing the particle size is necessary to improve simulation times. However, if the size increases are too large, the results may not be applicable for investigating realistic particle behaviour.

To investigate possible scaling effects, four different particle mixtures with different particle sizes will be simulated: three uniform particle sizes with diameters of 1 mm, 2 mm, and 3 mm as well as a graded sand with 25 mass-% of 1 mm, 50 mass-% of 2 mm, and 25 mass-% of 3 mm particles. Next to this variation in particle size, the scaling of different components necessary for the pluviation will also be considered in several simulations. To evaluate if the simulation results are realistic, they will be, where possible, compared to physical experiments conducted with an artificial, homogenous sand.

2 PHYSICAL AIR PLUVIATION

2.1 Design of the comparison experiments

Air pluviation is a method in geotechnics, to create homogenous sand samples of different densities. Here, a sand rain over a sample surface is created. The falling particles compact the particles below by transferring impact force. The main factors effecting the achieved densities as well as ensuring the desired homogeneity are the falling height, the deposition intensity (the amount of sand which falls on the sample surface per area and time) as well as the general set-up of the pluviation apparatus [5]. Therefore, both physical and numerical modeling of the process need to be variable in these aspects. To achieve this variability, the physical pluviation apparatus used for this research consists of the following components: a silo, a slide dampener, a chamber with calming trays, a sieve, two diffusor sieves and a sample container.

The silo contains the sample before the experiment. At the start of the experiment, the slide dampener is opened. From there, the sand passes two calming trays before reaching the sieve. The calming trays are two sieves with an open surface area of 30 %. This means, that 30 % of the area of the calming trays is covered in openings. They are responsible for ensuring a mixed sample over the sieve. This is necessary due to possible grain size separation of the sand sample while filling the silo. The sieve underneath the calming trays is responsible for regulating the deposition intensity of the sample by varying the open surface as well as the diameter of the openings. Underneath the sieve different diffusor sieves are attached. They distribute the sand equally over the sample surface. The last component of the pluviation apparatus is a sample container, which is placed at a specific height underneath the sieve. The complete pluviation apparatus in comparison to the simulation can be seen in figure 1. With this set-up, several aspects of the pluviation process have been investigated in preliminary experiments, including the influence of grain size and partial vacuum.

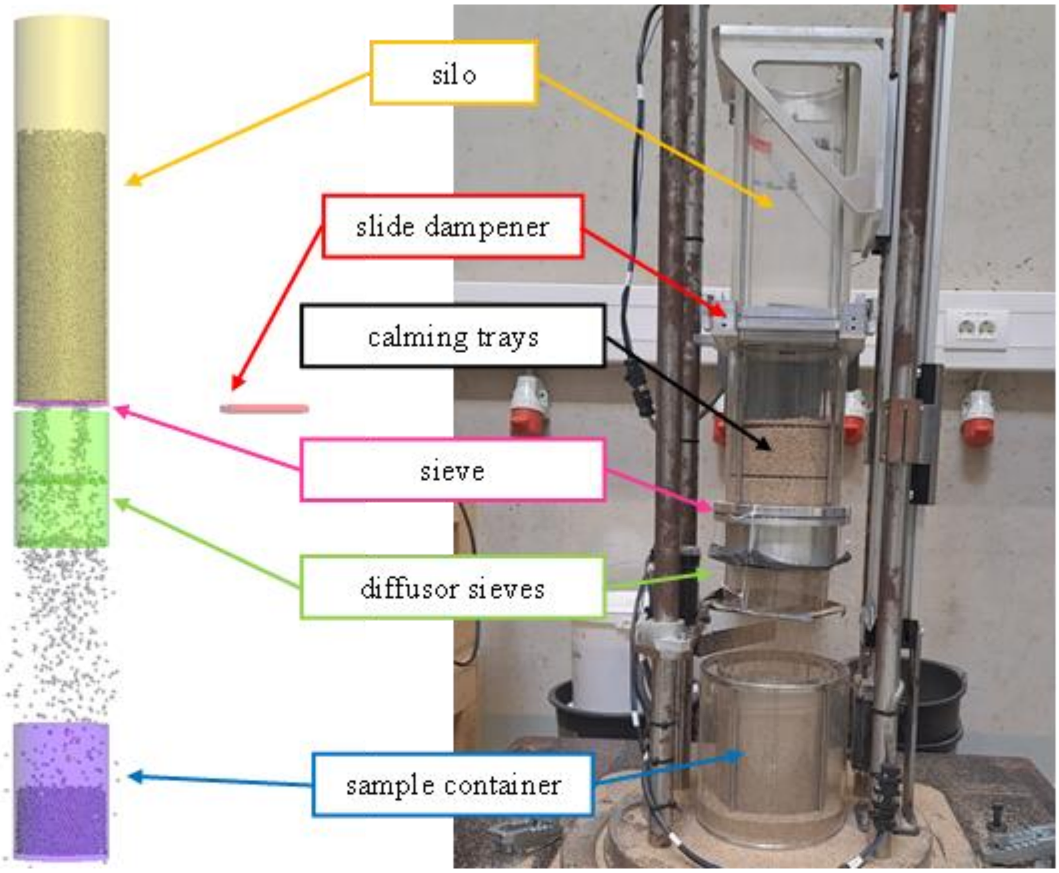

Figure 1: Comparison of numerical model (left) and physical model (right) of air pluviation simulation

For the comparative experiments a sieve opening of the pluviation apparatus of 10 % with an opening diameter of 4 mm was used. The two diffusor sieves consisted of a quadratic mesh with a mesh distance of 6 mm. The first diffusor sieve was attached 60 mm below the sieve, while the second was attached 50 mm underneath the first. The mesh was rotated by 45° between the two diffusor sieves. Recommendations for the diffusor sieve construction were taken from literature [5]. During the pluviation process, the pluviation apparatus was not lifted, so the falling height measured from the sieve varied from 400 mm to 200 mm while the sample was filled.

2.2 Artificial sand

The experiments for comparison with the DEM simulations were conducted with an artificial sand. It was created by sieving a natural sand, so 95,5 % of the grains were between 1 mm and 0.5 mm. Due to dry sieving, 4,1 % of particles were between 0,5 mm and 0,4 mm. The median grain size was calculated to be 0,74 mm, however, the accurate value for the median grain size could not be determined by sieving due to the limited amount of sieve sizes. The main component of the sand was quartz. During preliminary experimentation, the angle of repose of the sand was determined to be 29,1°, with straight or slightly convex slopes and a slightly rounded top. A picture of the angle of repose can be seen in figure 2.

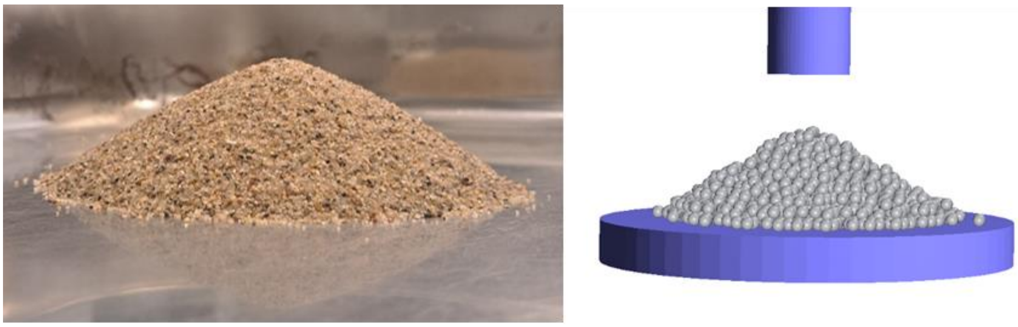

Figure 2: Comparison of physical angle of repose and simulated angle of repose (particle size 3 mm, parameter calibration complete)

2.3 Experimental results

During the comparative experiments, an average density of 1.690 g/cm³ and an average porosity of 0.362 could be determined for the described pluviation set-up and sand. Further, two empirical results could be achieved. These were important to evaluate how well different simulated particle sizes could depict the processes involved in air pluviation.

First, the openings in the sieve need to be large enough to allow for unrestricted flow of the sand. If the openings are too small, the internal friction of the particles does not allow the sand to fall. This was the case for an opening size of 3 mm (which would equal a ratio of three for the sieve opening diameter and the maximum particle size). Here, only a very small amount of sand particles fell before the particle flow was stopped. This phenomenon could be attributed to arching of the sand particles above the sieve openings. Therefore, a larger sieve opening diameter of 4 mm (ratio of opening diameter/maximum particle size of four) was used. With this configuration, no arching or inhibited flow was detected.

Secondly, the chosen diffusor sieves could adequately distribute the sand across the sample surface. While the individual interactions of singular grains with the diffusor sieves could not be observed, the diffusor sieves should, to maintain homogenous conditions, distribute the sand equally in all directions, while creating an even velocity distribution of the particles.

3 GERNERAL DESCRIPTIONS OF THE DEM-SIMULATIONS

3.1 General simulation framework

For all following simulations similar boundary conditions were used. The program used for the DEM simulations is the free code MUSEN [6]. The simulation time step was calculated using Rayleigh time [7] rounded to one significant digit. If there were multiple different time steps recommended due to different particle sizes, the smallest time step was chosen. The contact model used was Hertz-Mindlin, a contact model often used for DEM simulations [8].

Furthermore, to allow for a simplified simulation, only one other material (steel) was used besides the simulated sand. The important simulation parameters are summarized in table 1 and were unchanged during the simulations. For properly simulating the pluviation processes, these parameters would have to be calibrated as well. However, during these preliminary simulations, the given estimates should still be able to generally show the scaling effects.

Table 1: Material properties used in the simulation

Parameter	Unit	Value
Material properties of steel		
Density	kg/m³	7800
Young’s modulus	Pa	$2.1 * 10^{11}$
Poisson ratio	-	0.285
Interaction properties of steel on steel		
Restitution coefficient	-	0.8
Sliding friction	-	0.2
Rolling friction	-	0.05
Interaction properties of steel on sand		
Restitution coefficient	-	0.6
Sliding friction	-	0.5
Rolling friction	-	0.1

To depict all important aspects of the pluviation process the parameter calibration of the sand, the flow from the sieve, specifically, the necessary sieve opening diameter, the interactions of the diffusor sieves and the complete pluviation process will be simulated. All partial aspects will be simulated with the described particle sizes of 3 mm, 2 mm, 1mm as well as graded sand. Further, the sieve openings and the size of the diffusor sieves will also be varied, to determine what scaling factor is required to properly depict the physical experimentations.

3.2 Simulation limitations

Due to the simplification of the air pluviation process in DEM simulations, several limitations on the general applicability on further simulations apply.

First, the lack of air resistance in the numerical simulations could affect the particle behaviour. However, at the particle size, fallings height and deposition intensity used during the comparative experiments, the effect of air resistance should be negligible on the aspects considered for the numerical simulations. Secondly, the particles in the simulation were modelled as spheres. The sand grains used in the experiments however varied, reaching from rounded with high sphericity to subangular with medium sphericity. The changed shape will affect particle interactions with different components of the pluviation apparatus. The severeness of this effect is not known until now. Lastly, the restriction to only one material also influences the interactions of particles in the simulation. The physical pluviation apparatus consist of many different materials, such as acryl glass, aluminum, and different steels, which are not represented in the simulation.

However, despite these restrictions, the influence of particle scaling should still be detectable using the described simulations. The determined insights on the effects of particle scaling would also allow for further investigations on the reduction of the above-mentioned restrictions.

4 PARAMETER CALIBRATION

4.1 Simulation description

Parameter calibration is the first step during most numerical simulations. For the DEM simulation of air pluviation, particle interactions, and therefore friction and restitution coefficient are the most important parameters. Further, Young’s modulus and Poisson’s ratio also influence the packing density. However, these influences would be more important in larger reconstituted samples. Therefore, only the parameters restitution coefficient, sliding friction and rolling friction will be calibrated in this paper. For the Young’s modulus and the Poisson’s ratio approximate values from literature (such as [9]) and experiences from previous simulation are used. This also applies to the density of the particles, where simplified the density of quartz with 2650 kg/m³, the most common mineral in the experimental sand, is used.

One important note regarding parameter calibration of sand, is that it is a heterogeneous material. This does not only apply to the size and shape of sand grains, but also to the different minerals found in sand. Therefore, any parameters determined by parameter calibration should be considered as averages which only apply to a singular sand. Even changing the considered particle size or the source of the sand will change the parameters used for the simulations.

Because the parameter calibration mainly focuses on friction, the comparison to the angle of repose was used for evaluation purposes. Both, the achieved angle, and the shape of the cone, are important for the parameters. The simulation was created by simplifying the funnel used in the physical experiments as hollow cylinder. Inside this cylinder, the sand particles were randomly generated. The diameter of this cylinder was adjusted according to the investigated particle size. For 3 mm, 2 mm and the graded particles, the diameter of the cylinder was set to 20 mm, while for the 1 mm particles, it was reduced to 7 mm. Otherwise, it was not possible to avoid a flat top of the sand cone for the test with smallest particle size. The angle of repose was created on a flat cylinder. Both geometries funnel and flat cylinder were simulated as steel. To allow for an angle of repose to form, the hollow cylinder was slowly lifted from the flat cylinder.

To save simulation time, the first parameter calibration was for the particle size 3 mm, before calibration for other particle sizes were executed. Of specific interest was, if or how far the change in particle size effected the results of the parameter calibration, and if different particle sizes require different parameters for further simulations.

4.3 Results

For the particle size of 3 mm, appropriate parameters could be found after eight simulations. Here, both, the value and the shape of the angle of repose, matched the sand used for the comparative experiments. In the simulation, the angel of repose was 29,17°, which is very close to the one determined by the physical experimentation. Further adjustments to the parameters could not improve the simulation results. A comparison of the physical with the simulated angle of repose can be seen in figure 2.

By considering these parameters in the simulations with the other investigated grain sizes, only small changes could be found. While the shape of the angle of repose did not change with decreasing grain size, the value of the angle of repose had small variations. For the 2 mm sand the angle of repose was 29,45° while for 1 mm it was 28,74°. However, both variations were still in the range of values found during the physical experiments. Another factor affecting the variation in parameters could be the number of particles used. Too few particles reduce the simulation accuracy, especially when simulating larger particles. The same results could be found for the graded sand. Further changes of the simulation parameters did not improve the value of the angle of repose for any particle size. Because of this, it was decided to use one set of parameters for all further simulations, which is summarized in table 2.

Table 2: Material properties of the calibrated sand used for further simulations

Parameter	Unit	Value
Density	kg/m³	2650
Young’s modulus E	Pa	$5 * 10^9$
Poisson’s ratio ν	-	0.2
Restitution coefficient e	-	0.70
Sliding friction	-	0.25
Rolling friction	-	0.12

5 INFLUENCE OF SIEVE OPENING DIAMETER

5.1 Simulation set-up

Interactions with sieve openings were early on identified as one of the largest concerns in creating the simulations. The arching phenomenon during the experimentation results, described in section 2, was significant during preliminary simulations, especially with larger particle sizes. Therefore, the sieve opening diameter needs to be appropriately large. However, using sieves with the smallest possible opening diameters is preferable, because it allows for more sieve openings, which better distributes the sand over the sample.

To investigate the influence on the minimum ratio of sieve opening diameter over particle size, three different ratios were simulated for uniform sand: three, five and seven. For graded sand, the same ratios were considered compared to the largest particle size in the sample. Furthermore, the ratio of six was also investigated for 3 mm uniform sand.

5.2 Simulation results

During the simulation, three different behaviours could be observed based on sieve opening size and particle size. The first phenomenon was complete arching over the openings. Here, only very few particles could fall before the openings were blocked. This happened for all investigated sands for sieve opening diameters only three times as large as the largest particles. The second phenomenon was partial arching, where only a fraction of the openings experienced arching, or where times of arching and times of no arching occurred, leading to an intermittent flow. This concerned mainly the ratio of five times the particle size for the sieve opening for the simulation of uniform sands. The third option was that no arching occurred. This was the case for all sands in simulation with a ratio of seven as well as for the graded sand for a ratio of five. It also applied to the 3 mm sand at a ratio of six. Here, the flow of the sand particles out of the sieve was unobstructed. An example of the described behaviours can be seen in figure 3.

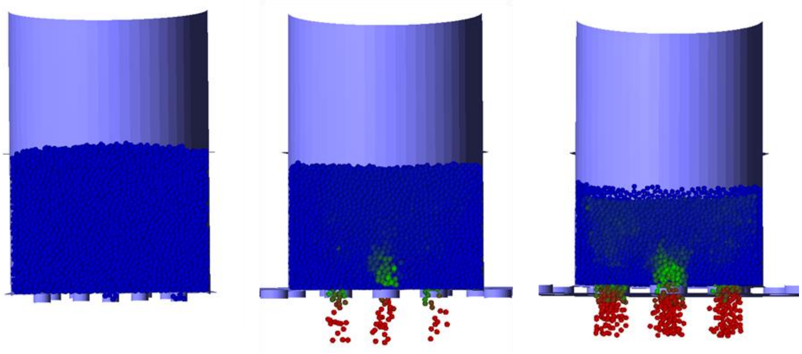

Figure 3: Outflow of 2 mm uniform particles out of sieve openings with diameters of 6 mm (left), 10 mm (middle) and 14 mm (right), colored by velocity (from 0 m/s to 0.5 m/s)

5.3 Comparison to Experimentation

The results of the numerical simulations were partially similar to the results achieved through physical experimentation. During the physical experimentation, a ratio of sieve opening diameter to maximum grain size of 3 lead to complete aching, which was replicated in all numerical simulations. However, while for a ratio of four during the physical experiments no arching could be detected, the same could not be said for the simulation with uniform grain sized sands. Here, partial arching occurred even with a ratio of five. Only by further increasing the sieve openings to seven times the particle size, no arching could be detected. For the graded sand, the behaviour was more similar to the behaviour of the real-world sand. Here, no arching could be detected starting from a ratio of sieve opening diameter to maximum particle size of five.

Therefore, creating variations in particle size seems to better depict the interactions with the sieve openings, which lead to the arching phenomenon. If, however, the simulation is conducted considering uniform particles, the sieve openings will need to be enlarged. This will be considered in the further simulations to allow for an unobstructed flow of the sand particles.

6 INTERACTIONS WITH DIFFUSOR SIEVES

6.1 Simulation set-up

To investigate the interactions of the grains with the diffusor sieves, not only the particle size, but also the size of the diffusor sieve meshes needs to be considered. Therefore, three different mesh sizes for the diffusor sieves are considered: a 6 mm x 6 mm quadratic mesh, which corresponds with the real-world size of the diffusor sieves, a 12 mm x 12 mm mesh, which is twice as large, and a 20 mm x 20 mm mesh, which is significantly enlarged. To replicate the construction of the diffusor sieves, the distance of 50 mm between the diffusor sieves and the rotation of 45° as used in the physical experiments are replicated in all simulations.

In the simulation the mesh material consists of steel. Due to the lack of parameter calibration for sand-mesh interaction, friction and partially elastic impacts are not properly simulated. However, the different scales will provide insights on how scaling of the simulation components effect the results.

6.2 Simulation results

Evaluating the simulation results by comparing them to specific aspects of the physical diffusor sieve interactions is rather difficult, because single interactions between particles and diffusor sieves can not be observed in the experiment. Therefore, the effectiveness of the diffusor sieves will be evaluated.

To achieve this, several aspects need to be considered. First, the diffusor sieves should be effective in distributing the particles evenly over the sample surface, since this was achieved during the experiments. Secondly, the velocity distribution of the particles should be uniform, both vertically and horizontally, to create homogenous compaction of the later sample. Finally, all particles need to be able to easily pass the diffusor sieves, so no plugging occurs. To better compare the different outcomes, both particle and velocity distribution of the simulations will be described as uniform, partially uniform or not uniform based on the achieved numerical results, see table 3.

Table 3: Results of the simulations of the diffusor sieves

Particle size	Diffusor mesh size	Particle distribution	Velocity distribution
3 mm	20 mm	Uniform	Partially uniform
	12 mm	Uniform	Uniform
	6 mm	Plugging of the diffusor sieve	
2 mm	20 mm	Partially uniform	Uniform
	12 mm	Uniform	Uniform
	6 mm	Nor uniform	Uniform
1 mm	20 mm	Not uniform	Not uniform
	12 mm	Not uniform	Not uniform
	6 mm	Uniform	Uniform
graded	20 mm	Uniform	Uniform
	12 mm	Partial plugging of the diffusor sieves	
	6 mm	Plugging of the diffusor sieves	

One specific point of interest are the differences between graded sand and uniform sand with 3 mm particles. While the 12 mm mesh created a uniform particle and velocity distribution for the 3 mm uniform sand, for the graded sand partial plugging of the diffusor sieve could be detected. This was due to the fact, that 3 mm particles collided more often with the diffusor sieves than smaller particles, leading to a seemingly small accumulation on the diffusor sieves. During the simulation with uniform particles, this phenomenon did not occur. The specific interactions with the graded sand and the diffusor sieves can be seen in figure 4.

Besides this effect, it can generally be seen that the size of the diffusor should be enlarged at the rate or slightly smaller than the particle size. Special attention however needs to be paid to the scaling if particles with different sizes are simulated. Here, scaling of the diffusor sieves should occur at the rate of particle scaling to avoid uneven particle distribution.

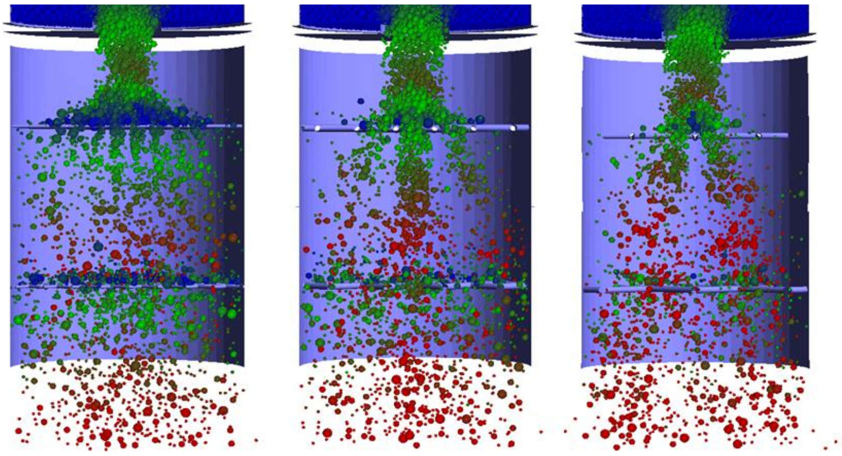

Figure 4: Interactions of graded sand with diffusor sieves mesh of 6 mm (left), 12 mm (middle) and 20 mm (right), colored by velocity (0 m/s to 1 m/s)

7 FULL SIMULATIONS OF PLUVIATION PROCESS

7.1 Simulation set-up

Simulating the full pluviation process allows for the investigation of all influences on the air pluviation process, including a comparison with or the prediction of the achieved densities. The simulations can also be used to identify reasons for inhomogeneity. Thus, the simulation needs to be as close as possible to the real-world situation. However, some simplifications are possible. As the simulated sands are either uniform or randomly created in the silo, the calming trays for mixing the sample over the sieve are not required. Therefore, they are omitted in the simulation as the effect should be negligible. The simulation set-up in comparison to the physical experiments is shown in figure 1.

Due to long simulation times the simulated pluviation had to be scaled down. This concerned both diameter of the entire set-up, which was reduced by two, as well as the height of the sample container. Based on this and the above observations, the design of the different simulation is summarized in table 4.

Table 4: Scaling used for the simulations of the complete air pluviation process

Particle size	Sample height ratio	Sieve Opening	Diffusor mesh size
3 mm	1:2	18 mm	12 mm
2 mm	1:2	12 mm	12 mm
1mm	1:4	6 mm	6 mm
graded	1:4	18 mm	20 mm

7.2 Simulation results

The comparison of the results of physical experiments and numerical simulations can be seen in table 5. Although all simulations show a difference between sample porosity and experimental porosity, some trends can still be observed. First, the achieved density improves between the particle sizes 3 mm and 2 mm, when it nears the particle size in the experiment. However, this improvement does not continue with 1 mm particle size. Here, the density does not further improve. This, however, could be the result of the reduced sample height for this simulation. Another factor that affects the results is grading of the particles used. For graded particles used in the simulation, the density was overestimated, while for the uniform sands it was underestimated. This might be due to the higher compaction ability of sand which are more graded compared to those which are not [10]. This would mean, that grading of the sand simulated should be depicted as best as possible to achieve realistic simulation results.

Table 5: Results of air pluviation simulations in comparison to experiments

Particle size	Average density [g/cm³]	Average porosity [-]	Deviation to comparison porosity [-]	Computational time[h] for 1 s simulation time
Comparison experiments	1.690	0.362	NA	NA
3 mm	1.627	0.386	+ 0.024	2.13
2 mm	1,648	0.378	+ 0.016	11.47
1 mm	1.632	0.384	+ 0.022	12.33
graded	1.754	0.338	- 0.024	10.833
graded-new	1.683	0.365	+ 0.003	3.80

To test this, another graded sand (graded-new in table 5) was simulated. Its grading, consisting of one-third particles of 2 mm, 3 mm, and 4 mm each was able to predict the achieved density and porosity significantly better, even while using a large particle scaling. Thus, for future simulations, grading of simulated particles should closely match the physical sand used.

8 CONCLUSIONS

Based on the conducted simulations, it is possible to achieve realistic results from the DEM simulation of air pluviation, even when increasing particle size. However, certain requirements need to be considered for achieving evaluable results.

First, parameter calibration of inter-particle friction is not or only very limited affected by scaling of the particles. However, the applicability of this to other parameters like Young’s modulus or the Poisson’s ratio still need to be determined. This applies to uniform as well as graded particles, so no scaling needs to occur here.

However, to mimic interactions between the particles and the components of the pluviation apparatus, the size of the components will need to be increased along with the particle size. The scaling factor here is influenced by the grading of the sand. The more similar the grading of the experimental sand is to the sand used for the numerical modelling, the more similar the scaling factor is. This also applies to the achieved densities in the simulation, which are less effected by the actual scaling of the particle size, but more by the grading of the particles in the simulations.

With these insights, it is possible to scale up particles for further simulations. This will drastically reduce the necessary computational times and simplify future investigations of the pluviation process.

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