Effects of grain size and shape distributions on the critical strength of granular materials: a DEM study.

Estudio DEM sobre el efecto de la dispersión de tamaño y forma de partículas en la resistencia critica de materiales granulares.

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ABSTRACT: The shear strength of coarse granular materials, such as rockfills or mine waste rocks, is typically evaluated on small samples by adjusting the particle size distribution (PSD) of the field material. While the peak friction angle depends on the PSD and state properties, extensive experimental evidence shows that the critical friction angle remains unaffected by PSD changes if particle shape and roughness are constant across different sizes. However, correlations between grain size and shape in crushed rocks could impact the material properties, raising questions about the representativity of scaling methods. This study uses 3D discrete element simulations to investigate the effects of grain size and shape distributions on the critical strength of granular materials. Numerical tests are carried-out on samples having diverse grain shapes (from spheres to polyhedral) and varied PSDs. The findings reveal that size/shape correlations can significantly influence the critical shear strength. The conclusions emphasizes that both grain size and shape distributions should be measured in order to verify the validity of scaling methods on a given coarse granular material.

KEYWORDS: small-scaling, shear strength, discrete-element modeling, grain size, grain shape.

1 INTRODUCTION.

Stability analyses of rockfill dams, mine waste rock dumps, or gravel dikes require shear strength properties of coarse granular materials, often involving oversized particles that can not be accommodated in laboratory devices (Marsal, 1967; Marachi, 1972; Verdugo & De la Hoz, 2006; Ovalle et al., 2020). To address this challenge, engineers perform shear tests on small-scaled samples prepared through techniques such as scalping or parallel grading. Despite extensive reported research on the impact of these methods on the material shear strength, results vary considerably and are often contradictory. While some studies suggest a decrease in shear strength with grain size (Marachi et al., 1972; Ovalle et al., 2014; Xiao et al., 2014), others indicate the opposite trend (Al-Hussaini, 1983; Varadarajan et al., 2003; Cao et al., 2020). These inconsistencies likely arise from differences in inherent material properties (e.g., grain shape and roughness, grain crushing strength) and state properties (e.g., moisture, relative density). To have a better understanding of these empirical apparent contradictions, this study focuses on the effects of particle shapes and sizes on the mechanical behavior of granular materials.

Adjusting the particle size distribution (PSD) during small-scale sample preparation can impact packing density and, thus, peak strength. On the other hand, it is well known that the critical Mohr-Coulomb friction angle is independent of PSD, provided that particle shape and surface roughness remain constant through grain sizes (Muir Wood & Maeda, 2008; Voivret et al., 2009; Li et al., 2013; Cantor et al., 2018; Yang & Luo, 2018; Cantor & Ovalle, 2023; Ovalle et al., 2023; Polanía et al., 2023, Girumugisha et al. 2024). Nevertheless, recent studies show that particle shape could be correlated to grain size (size-shape correlations) through sedimentary lamination or fine foliation induced by metamorphism in certain rockfill materials (Linero et al., 2017). Shearing tests on materials having particle size-shape correlations exhibit notable differences in critical shear strength for scaled PSD (Ovalle & Dano, 2020), which has also been analyzed through numerical Discrete-element modeling (DEM) simulations (Linero et al., 2019; Carrasco et al., 2022, 2023).

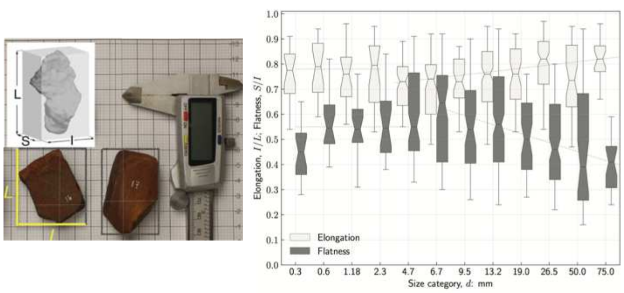
DEM is a numerical approach used to simulate the behavior of granular materials by representing individual particles as discrete entities and modeling their interactions (Cundall & Strack, 1979; Moreau, 1988). Despite its versatility, much of the existing DEM research predominantly relies on spherical particles due to computational convenience and the simplified treatment of contact mechanics. However, this prevalent focus on mono-shaped spherical grains constrains the representation of real granular materials. DEM studies utilizing non-spherical particles provide a valuable understanding of particle shape effects. However, they remain focused on mono-shaped grains (Azema & Radjaï, 2012; Cantor et al., 2018, 2020; Kawamoto et al., 2018). This research takes a step forward in this topic by incorporating assemblies composed of particles with a diverse range of shapes, including spherical and polyhedral particles. The study explores the coupled effects of grain size, shape, and PSD on the critical friction angle of granular materials. 3D-DEM triaxial shearing tests were simulated across various PSDs, and extensive analyses were carried out on the macro-mechanical behavior under critical state conditions.

2 SIZE-SHAPE CORRELATIONS

2.1 *Size-shape correlation on granular materials*

Natural and industrial granular materials often exhibit polydispersity in grain sizes and shapes, as highlighted in recent studies (Linero et al., 2017; Zhao et al., 2023). PSD analyses typically quantify the abundance of particles based on their size and mass. However, crucial information regarding particle shape should be analyzed separately, which includes characteristics such as angularity, elongation, and flatness.

As shown in Figure 1a, Linero et al. (2017) defined the following particle shape descriptors: (i) elongation, denoted by the ratio of breadth to length (I/L), and (ii) flatness, defined as the ratio of thickness to breadth (S/I); where L represents the greatest distance between two parallel planes tangential to the particle surface, I is the maximum dimension perpendicular to L, and S denotes the maximum dimension perpendicular to both L and I. For a colluvial material that Linero et al. (2017) investigated, Figure 1b illustrates a trend in particle shape across particle sizes: coarser particles tended to be flatter than finer grains.



(a) (b)

Figure 1. (a) Particle characterization and (b) size-shape correlation in terms of particle elongation and flatness (Linero et al., 2017).

As shown in Figure 2a, Ovalle & Dano (2020) assessed particle shape through measurements of L and I on individual particles. Employing the parallel grading small-scaling method, they generated three parallel PSDs with varying maximum particle diameters (d_{max}): 10 mm (STV0), 40 mm (STV1), and 160 mm (STV2). Figure 2b presents data illustrating the average grain elongation as a function of particle size. Their findings corroborate a particle size-shape correlation within the STV material: as particle size increases, the average elongation rises while the standard deviation decreases. Consequently, finer particles tend to exhibit higher elongation and greater variability in shape. As presented in Figure 2c in terms of the Mohr-Coulomb internal friction angle (ϕ), the scaling method modifies ϕ, presumably due to different characteristic particle shapes between samples STV0, STV1, and STV2.

2.2 *Simulated granular material*

To investigate the influence of size and shape dispersion on granular materials, particle assemblies exhibiting a size-shape correlation determined by angularity are prepared in this study. The angularity of regular polyhedral particles is characterized by the number of vertices (n_v) or the number of faces (n_f), which are related by $n_f = 2\,n_v - 4$. These vertices are connected by a convex hull, resulting in the formation of regular polyhedra.

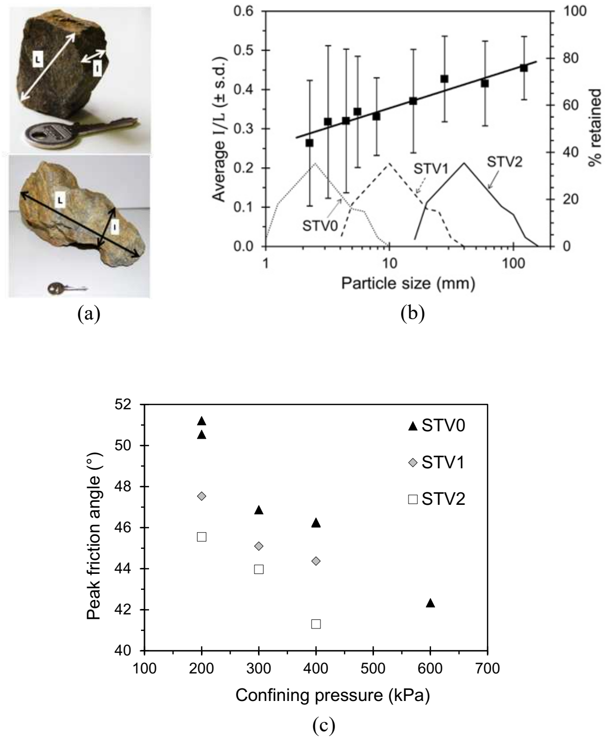


Figure 2. (a) Particle characterization, (b) size-shape correlation, and (c) internal friction angle (Ovalle & Dano, 2020).

The variety of particle shapes included regular octahedral forms (with n_v= 6) to spheres. The characteristic size of a particle is defined as the diameter (d) of the circumscribed sphere that envelops its convex hull, as shown in Figure 3. The particle sphericity is computed by the following expression:

$$\Psi = \frac{V_P}{V_S} \tag{1}$$

where V_P is the volume of each particle, and V_S is the volume of the circumscribing sphere. Table 1 shows the geometrical characteristics of the simulated particles.

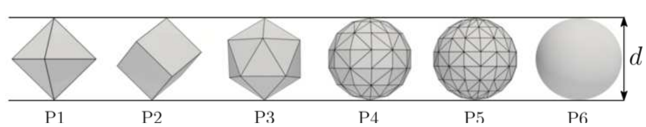


Figure 3. Numerical particle shapes.

We present two size-shape correlations based on previously described grain shapes. In *Case A*, larger grains have higher sphericity, while smaller grains tend to be more angular. Conversely, in *Case B*, larger grains have angular shapes, whereas smaller grains exhibit higher sphericity. Note that samples for Case A and Case B can have the same PSD, but different size/shape correlations. To quantify the variation in the PSD, we used the coefficient of uniformity $C_u = D_{60}/D_{10}$ as a quantitative measure. Figure 4 illustrates all PSD used in this study, varying from mono-size samples ($C_u = 1$) to relatively size dispersed samples ($C_u = 2.6$); d_{max}/d_{min} ranges from 1 to 6, respectively.

Table 1. Geometrical characteristics of the grains.

Particle	n_v	n_f	Ψ
P1	6	8	0.32
P2	8	12	0.37
P3	12	20	0.61
P4	74	144	0.91
P5	130	256	0.95
P6	Spheres	-	1

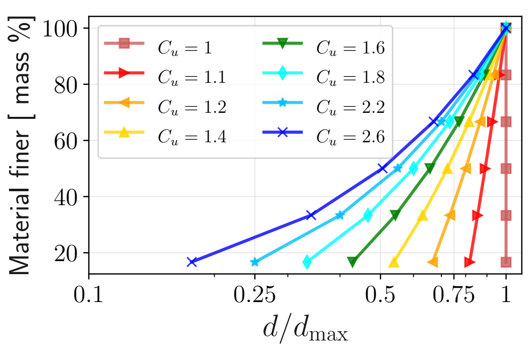


Figure 4. Particle size distributions of different C_u.

2.3 Sample generation and shearing tests

We set a maximum particle size (d_{max}) to 15 mm and create granular arrangements based on specified PSDs and correlations between size and shape. Particles are placed into layers using a geometrical protocol, forming assemblies of between 10 000 to 15 000 grains. These depositions take place within a rectangular container of width (W) and height (H), resulting in samples as in Figure 5(a). Importantly, our box dimensions comply with the international testing standard ASTM D7181, so that $H/W = 2$ and $W/d_{max} \geq 7$.

The interaction between grains was simulated using a dry frictional contact model, with a constant coefficient of friction (μ) set to 0.4. The friction coefficient (μ) was set to zero for wall-particle interactions, while gravity was disabled to eliminate pressure gradients within the system. The density of the grains is set to 2700 kg/m³. The shearing tests were conducted using LMGC90, an open-source platform renowned for its ability to simulate discrete mechanical systems (Dubois et al., 2011). LMGC90 employs the Non-smooth Contact Dynamics (NSCD) method, allowing for an accurate representation of granular interactions and facilitating the incorporation of diverse 3D particle shapes into the simulations (Radjai & Richefeu, 2009). This robust computational framework enables the analysis of granular behavior under controlled shearing conditions, contributing to a deeper understanding of the mechanical response of granular materials.

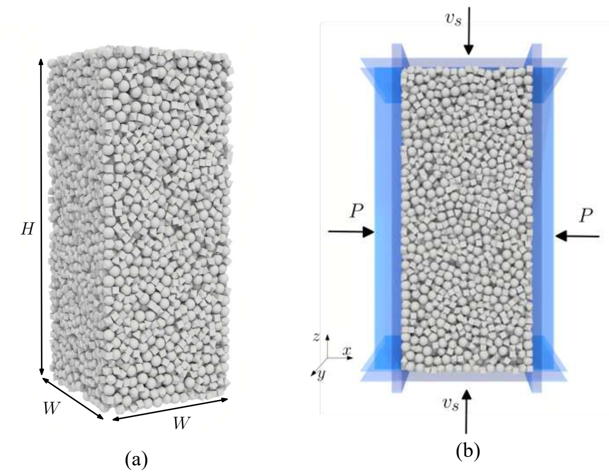


Figure 5. (a) Dimensions of the rectangular sample ($C_u = 1$) and (b) drained triaxial shear test configuration.

The granular samples first undergo compression via an isotropic pressure of 10 kPa after deposition. This compression is achieved by applying controlled forces to rigid walls on all the faces of the sample box, ensuring uniform compaction throughout the assembly. Figure 6 presents zoom-in snapshots of the samples after isotropic compression, showcasing distinct packing configurations for different size-shape correlations and uniformity coefficients. Figure 5(b) shows drained triaxial shear tests configuration. These tests are conducted by applying a constant velocity (v_s) to both the upper and lower walls of the samples, while lateral walls maintain constant confinement stress of 10 kPa. The shearing rate is determined based on the inertial number ($I = 10^{-3}$), allowing for quasi-static shearing conditions (GDR-MiDi, 2004). Samples are sheared until reaching an axial deformation of $\varepsilon_a = 0.4$.

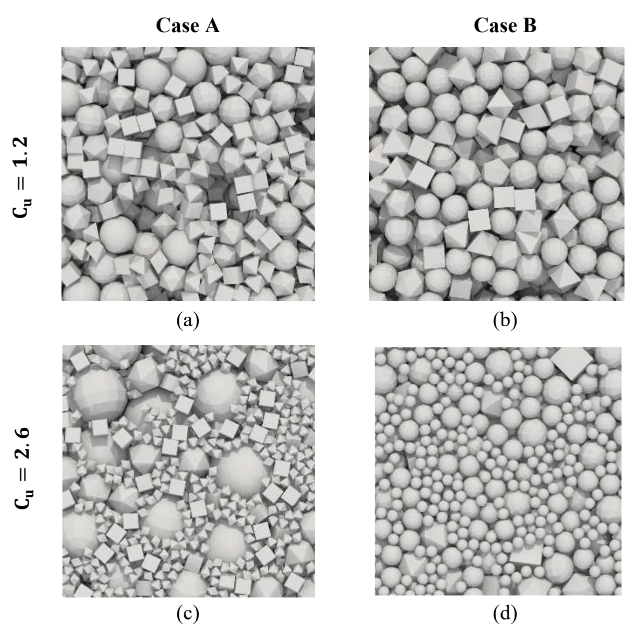


Figure 6. Zoom-in screenshots of samples with particle size span C_u=1.2 (top) and C_u=2.6 (bottom) for both size-shape correlation.

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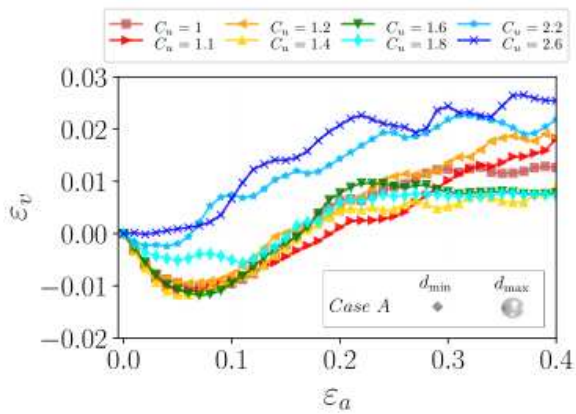
3 RESULTS

3.1 *Shearing test results*

Figure 7 shows the volumetric strain (ε_v) as a function of ε_a. It is worth noting that at lower levels of axial deformation, samples with low C_u show an initial contraction phase between $\varepsilon_a = 0$ to 0.1, followed by dilatation. However, as the deformation progresses, all samples reach a critical volumetric strain after $\varepsilon_a = 0.3$.



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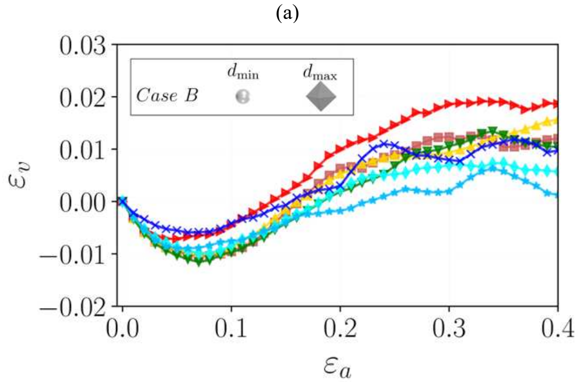

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Figure 7. Evolution of the volumetric strain ε_v as a function of axial deformation ε_a

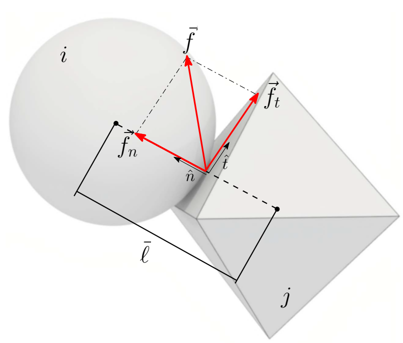


Figure 8. The local frame of contact between particle i and j.

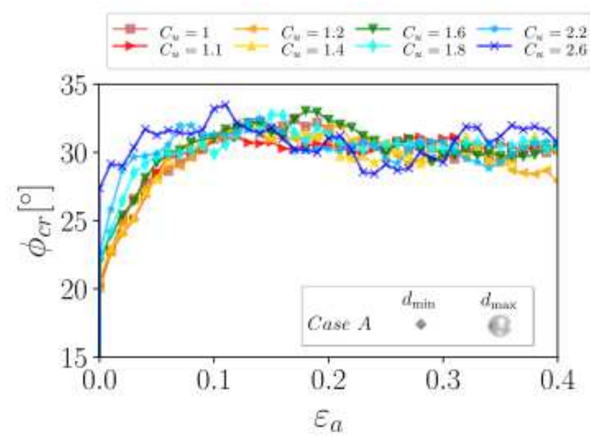
The stress state is characterized by the deviatoric stress $q = (\sigma_1 - \sigma_3)$ and the mean stress $p = (\sigma_1 + \sigma_2 + \sigma_3)/3$, computed from the granular stress tensor σ_{ij} defined as (Rothenburg & Bathurst, 1989):

$$\sigma_{ij} = \frac{1}{V} \sum_{\forall c} f_i^c \, \ell_j^c \,, \tag{2}$$

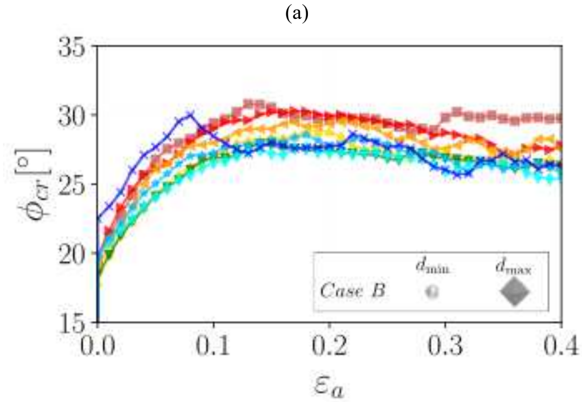
f_i^c denotes the i component of the force at contact c and ℓ_j^c is the j component of the branch vector, which joins the center of mass of touching particles at contacts c (see definitions in Figure 8). In triaxial configuration, the normalized shear stress at critical state ($M = q/p$) has a direct relationship with the critical state friction angle of the material (ϕ_{cs}) as:

$$\sin \phi_{cs} = \frac{3\,M}{6+M} \tag{3}$$

Figure 9 displays the evolution of ϕ_{cs} upon shearing. It can be observed that ϕ_{cs} stabilizes across all samples after ε_a = 0.2. Notably, assemblies with rounded fine particles (Case B) exhibit lower fluctuations in shear strength than their counterparts (Case A). In terms of stress response, all samples exhibit critical state behavior after ε_a = 0.3.



(a)



(b)

Figure 9. Evolution of ϕ_{cs} as a function of axial deformation ε_a

3.2 *Effects of size-shape correlation on critical state condition*

Figure 10 presents the evolution of ϕ_{cs} against C_u for both Case A and Case B scenarios. Case A, characterized by fine angular grains and larger spherical particles, exhibits a relatively constant ϕ_{cs} of around 30 degrees as C_u increases. In contrast, Case B, featuring spherical fines and larger angular particles, shows a descending trend. However, as C_u increases, ϕ_{cs} decreases to 27 degrees for $C_u = 1.8$, before stabilizing for larger values of C_u. The mechanisms behind these macro-mechanical observations lay at the micro-mechanical scale, that is, at the scale of the particles. As shown by Carrasco et al. (2022, 2023), fine angular grains in Case A promote interlocking by filling large pores between coarse rounded grains, thus significantly contributing to the material strength. On the other hand, rounded fine grains in Case B are more likely to float within large pores, without significant contribution to the intergranular force network, thus decreasing the material strength.

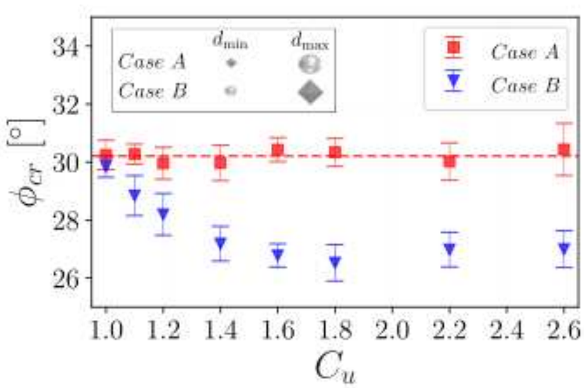


Figure 10. Evolution of critical friction angle ϕ_{cs} as a function of C_u for Cases A and B. Red dashed lines represent mean value for all samples of Case A.

4 CONCLUSIONS

Several studies have explored the shearing behavior of granular materials through samples with mono shaped particles. These mixtures have focused on the interaction between coarse angular material and rounded fine particles, consistently revealing a decrease in the critical friction angle ϕ_{cs} as the proportion of fine-rounded particles increases (Santamarina & Cho, 2004; Gong et al., 2024). However, a notable gap remains in understanding how a broader dispersion of particle shapes and sizes influences ϕ_{cs}. To address this, systematic studies employing materials with opposing size-shape correlations in both shearing tests (Carrasco et al., 2022, 2023) and dynamic run-out conditions (Nie et al., 2024) have recently been conducted. These studies highlight the role of fine particles in determining shear strength, especially when applying small-scaling techniques, where the small-scaled samples tested are comprised of the finest particles of the prototype material.

This paper presents a comprehensive investigation into the effects of granular assemblies characterized by correlations between the size and shape of the grains. This study spanned a wide range of granular configurations, including mono-size to polydisperse arrangements, with a maximum size ratio of approximately d_{max}/d_{min} =6. Utilizing the contact dynamics discrete element method, 3D granular assemblies under triaxial shearing were simulated up to a cumulated deformation of $\varepsilon_a = 0.4$.

In Case A, featuring a correlation between larger spherical grains and smaller angular grains, the shear strength remains relatively constant despite variations in grain size span. Conversely, in Case B, characterized by the opposite size-shape correlation, shear strength gradually decreases as the grain size span increases. These finding complemented by Carrasco et al. (2022, 2023), can explain the decrease on peak friction angles as d_{max} increases reported by Ovalle and Dano (2020). The reduction in d_{max}, achieved through various parallel PSDs, results in a higher proportion of fine, elongated, and angular particles within the samples. This shape modification enhances interparticle interlocking, thereby augmenting the shear strength. These results emphasize the importance of considering grain shapes in scaling methods, such as scalping or parallel grading. For instance, if a given material presents strong size-shape correlations, scaling methods will be limited and will involve changing the characteristic particle shape of the sample. Therefore, the scaling method will not be suitable for strength estimations. On the other hand, if particle shape is maintained across grain sizes, scaling should give consistent values of the critical friction angle.

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6 REFERENCES

Al-Hussaini, M. (1983). Effect of particle size and strain conditions on the strength of crushed basalt. *Can. Geotech. J.*, *20*(4), 706–717.

Azema, É., & Radjaï, F. (2012). Force chains and contact network topology in packings of elongated particles. *Physical Review E*, *85*(3), 031303. https://doi.org/10.1103/PhysRevE.85.031303

Cantor, D., Azéma, E., Sornay, P., & Radjai, F. (2018). Rheology and structure of polydisperse three-dimensional packings of spheres. *Phys. Rev. E*, *98*(5), 052910.

Cantor, D., & Ovalle, C. (2023). Sample size effects on the critical shear strength of granular materials with varied gradation and the role of column-like local structures. *Géotechnique*., 1-12.

Cao, P., Jiang, M., & Ding, Z. (2020). Effects of particle size on mechanical behaviors of calcareous sand under triaxial conditions. *Jpn. Geotech. Soc. Spec. Publ.*, *8*(5), 182–187.

Carrasco, S., Cantor, D., & Ovalle, C. (2022). Effects of particle size-shape correlations on steady shear strength of granular materials: The case of particle elongation. *Int. J. Numer. Anal. Methods. Geomech.*, *46*(5), 979–1000.

Carrasco, S., Cantor, D., Ovalle, C., & Quiroz-Rojo, P. (2023). Shear strength of angular granular materials with size and shape polydispersity. *Open Geomechanics*, *4*, 1–14.

Cundall, P., & Strack, O. (1979). A discrete numerical model for granular assemblies. *Geotechnique*, *29*(1), 47–65.

Dubois, F., Jean, M., Renouf, M., Mozul, R., Martin, A., & Bagnéris, M. (2011). LMGC90. *10e Colloque National En Calcul Des Structures*, 8 p.

GDR-MiDi. (2004). On dense granular flows. *Eur. Phys. J. E*, *14*, 341–365.

Girumugisha, G., Ovalle, C., Ouellet, S. (2024). Sample Size Effect on Sh ear Strength of Mine Waste Rock Material Using the Scalping Method. Geo-Congress 2024, Vancouver, Canada, February 25 -28, 2024.

Gong, J., Pang, X., Tang, Y., Yang, Z., Jiang, J., & Ou, X. (2024). Effects of angularity and content of coarse particles on the mechanical behaviour of granular mixtures: A DEM study. *Granular Matter*, *26*(1), 17.

Kawamoto, R., Andò, E., Viggiani, G., & Andrade, J. E. (2018). All you need is shape: Predicting shear banding in sand with LS-DEM. *J. Mech. Phys. Solids*, *111*, 375–392.

Li, G. Ovalle, C. Dano, C. & Hicher, P.-Y. (2013). Influence of grain size distribution on critical state of granular materials. *Constitutive modeling of geomaterials.* 207-210.

Linero, S., Azéma, E., Estrada, N., Fityus, S., Simmons, J., & Lizcano, A. (2019). Impact of grading on steady-state strength. *Geotech. Lett.*, *9*(4), 328–333.

Linero, S., Fityus, S., Simmons, J., Lizcano, A., & Cassidy, J. (2017). Trends in the evolution of particle morphology with size in colluvial deposits overlying channel iron deposits. *EPJ Web of Conferences*, *140*, 14005.

Linero, S., Palma, C., & Apablaza, R. (2007). Geotechnical characterisation of waste material in very high dumps with large scale triaxial testing. *Proceedings of the 2007 International Symposium on Rock Slope Stability in Open Pit Mining and Civil Engineering*, 59–75.

Marachi, N., Chan, C., & Seed, H. (1972). Evaluation of properties of rockfill materials. *J. Soil Mech. Found. Div.*, *98*(1), 95–114.

Marsal, R. (1967). Large scale testing of rockfill materials. *J. Soil Mech. Found. Div.*, *93*(2), 27–43.

Moreau, J. J. (1988). Unilateral contact and dry friction in finite freedom dynamics. In *Nonsmooth mechanics and Applications* (pp. 1–82). Springer.

Muir Wood, D., & Maeda, K. (2008). Changing grading of soil: Effect on critical states. *Acta Geotech.*, *3*(1), 3–14.

Nie, J.-Y., Cui, Y., Wu, Z., Zhang, L., & Fang, J. (2024). DEM study on role of fines in mobility of dry granular flows considering particle size-shape correlation. *Computers and Geotechnics*, *166*, 105980.

Ovalle, C., Frossard, E., Dano, C., Hu, W., Maiolino, S., & Hicher, P. Y. (2014). The effect of size on the strength of coarse rock aggregates and large rockfill samples through experimental data. *Acta Mech.*, *225*(8), 2199–2216.

Ovalle, C., & Dano, C. (2020). Effects of particle size–strength and size–shape correlations on parallel grading scaling. *Géotechnique Letters*, *10*(2), 191–197.

Ovalle, C., Linero, S., Dano, C., Bard, E., Hicher, P.-Y., Osses, R. (2020): Data compilation from large drained compression triaxial tests on coarse crushable rockfill materials. *Journal of Geotechnica l and Geoenvironmental Engineering*. 146(9): 06020013.

Ovalle, C, Girumugisha, G, Cantor, D & Ouellet, S (2023). Size effects as sessment of mine waste-rock shear strength combining numeric al, laboratory and in situ approaches. *In PM Dight (ed.), SSIM 2023: Third International Slope Stability in Mining Conference* , Australian Centre for Geomechanics, Perth, pp. 291-300.

Polanía, O., Cabrera, M., Renouf, M., Azéma, E., & Estrada, N. (2023). Grain size distribution does not affect the residual shear strength of granular materials: An experimental proof. *Physical Review E*, *107*(5), L052901.

Radjai, F., & Richefeu, V. (2009). Contact dynamics as a nonsmooth discrete element method. *Mechanics of Materials*, *41*(6), 715–728. https://doi.org/10.1016/j.mechmat.2009.01.028

Rothenburg, L., & Bathurst, R. J. (1989). Analytical study of induced anisotropy in idealized granular materials. *Geotechnique*, *39*(4), 601–614.

Santamarina, J. C., & Cho, G. C. (2004). Soil behaviour: The role of particle shape. *Advances in Geotechnical Engineering: The Skempton Conference*, *1*, 604–617.

Varadarajan, A., Sharma, K. G., Venkatachalam, K., & Gupta, A. K. (2003). Testing and Modeling Two Rockfill Materials. *Journal of Geotechnical and Geoenvironmental Engineering*, *129*(3), 206–218.

Verdugo, R., & K. De la Hoz. 2006. "Strength and stiffness of coarse gran ular soils." *In Soil stress-strain behavior: Measurement, model -ing and analysis,* edited by H. I. Ling, 243–252. Dordrecht, Ne therlands: Springer.

Voivret, C., Radjaï, F., Delenne, J.-Y., & El Youssoufi, M. S. (2009). Multiscale Force Networks in Highly Polydisperse Granular Media. *Physical Review Letters*, *102*(17), 178001.

Xiao, Y., Liu, H., Chen, Y., & Zhang, W. (2014). Particle size effects in granular soils under true triaxial conditions. *Géotechnique*, *64*(8), 667–672.

Yang, J. and Luo, X. D. (2018). The critical state friction angle of granular materials: does it depend on grading?. *Acta Geotech*., 13:535–547

Zhao, J., Zhao, S., & Luding, S. (2023). The role of particle shape in computational modelling of granular matter. *Nature Reviews Physics*, *5*(9), 505–525.