

Article

Optimization of Discrete Element Method Model to Obtain Stable and Reliable Numerical Results of Mechanical Response of Granular Materials

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Abstract: The discrete element method (DEM) is largely used to simulate the geotechnical behavior of granular materials. However, numerical modeling with this type of code is expensive and time consuming, especially when fine particles are involved. This leads researchers to make use of different approaches to shorten the time of calculation without verifying the stability and reliability of numerical results, even though a compromise between the time of calculation and accuracy is commonly claimed. The particle size distribution (PSD) curve of studied granular material is completely ignored or arbitrarily cut. It is unclear if the ensued numerical results are still representative of the studied granular materials. Additionally, one can see a large number of numerical models established on a basis of calibration by ignoring the physical meaning and even measured values of some model parameters. The representativeness and reliability of the obtained numerical results are questionable. All these partly contribute to reducing the public's confidence in numerical modeling. In this study, a methodology is illustrated to obtain an optimal DEM model, which minimizes the time of calculation and ensures stable and reliable numerical results for the mechanical behavior of a waste rock. The results indicate that the PSD curve of the studied waste rock can indeed be cut by excluding a portion of fine particles, while the Young's modulus of the waste rock particles can also be decreased to accelerate the numerical calculations. A physical explanation of why the time of calculation can be shortened by reducing the Young's modulus of waste rock particles is provided for the first time. Overall, the PSD cut, reduction in Young's modulus, and time step must be determined through sensitivity analyses to ensure stable and reliable results with the shortest time of calculation. In addition, it is important to minimize the number of model parameters determined through the process of calibration, especially for those having physical meanings. In this study, the only model parameter having a clear physical meaning but difficult to measure is the rolling resistance coefficient for repose angle tests on the studied waste rock. Its value has to be obtained through a process of calibration against some experimental results. The validity and predictability of the calibrated numerical model have been successfully verified against additional experimental results.

Keywords: discrete element method (DEM); DEM model validation; optimal cut of PSD curve; optimal time step; optimal Young's modulus; predictability of DEM model



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1. Introduction

In several fields such as chemical engineering, powder engineering, and geotechnical engineering, one usually needs to deal with granular materials [1–6]. Over the years, one sees an increasing use of the discrete element method (DEM) [7] to analyze the mechanical behavior of granular materials in geotechnical engineering. The main advantage of the DEM is that the movements of individual particles, along with the interactions between particles, can be captured.

Despite the advantages of the DEM model compared to continua models, its application suffers from the requirement of huge and expensive sources of computation [8,9]. For

a poorly graded and coarse granular material, the narrow particle size distribution (PSD) curve can be readily reproduced by DEM models, and the time of computing can also be reasonable. For many cases, especially in geotechnical engineering with granular geomaterials like rockfill or waste rock, the PSD curves can be very wide, with fine particles as small as a few microns and coarse particle as large as several centimeters or even meters [10–15]. The numerical reproduction of the full PSD curve using the DEM model becomes extremely heavy, if not totally impossible. The time of computing can also be extremely long [16–18], even with powerful computing technologies, such as multi-graphical unit processors and parallel computing [19,20]. This partly explains the few and very limited applications of the DEM model to treat full-scale industrial problems in geotechnical engineering because the full consideration of the PSD curves of actual granular materials is still impossible [18,21].

Subsequently, an approach commonly adopted in DEM modeling is to exclude a portion of fine particles in an arbitrary way [22–26]. The computation time can be significantly reduced, but the stability, reliability, and representativeness of the obtained numerical results are questionable.

Another widely used approach to shorten the time of DEM computing is to reduce the stiffness of particles, rather than using the actual value of particle stiffness. Physically, reducing particle stiffness means that the simulated particles are softer than those of the actual material. The system could indeed reach a static equilibrium faster than that of the actual material. This explains why the time of calculation to equilibrium can be shortened. But the interactions between particles and the intermediate responses in terms of forces and deformation should be different from those of the actual materials. Surprisingly, several studies showed that the same results can be obtained by reducing the stiffness of particles [1,27–30]. If all these findings are true, can we reduce the value of particle stiffness to as small as a value close to zero? If not, what is the minimum value to ensure stable, reliable, and representative numerical results?

In DEM modeling, the time step is another factor that can affect the stability and reliability of numerical results. An excessively small time step leads to an unnecessarily long time of calculation, whereas an excessively large time step can result in unstable and unreliable numerical results [31,32]. An optimal time step should be determined to minimize the time of computing and to ensure stable and reliable numerical results [33]. However, it is seldom mentioned in published works on DEM modeling. Probably, the default time step value given in most DEM codes based on Rayleigh time is used [34–36]. It is, however, unclear if the default value is always optimal to minimize the time of computing and to ensure stable and reliable numerical results.

Finally, one notes that numerous DEM simulations were realized without making a distinction between calibration and prediction. In addition, few efforts were made to minimize the number of model parameters determined through the process of calibration. It is thus not rare to see the determination of some model parameters such as particle density, Poisson's ratio, static friction coefficient, etc. in an arbitrary way or through a process of calibration, even though these model parameters have clear physical meanings and can be readily obtained thorough laboratory tests. The uncertainty of the numerical model is high, and the credibility of the numerical results is low because good agreements between numerical and experimental results can be achieved by different combinations of these calibrated model parameters. All these factors, along with the previously mentioned practices, contribute to compromising the public's confidence in numerical modeling, a phenomenon quite special in geotechnical engineering [37].

In this study, a commercialized DEM code, named EDEM [38] was chosen to simulate the mechanical behavior of a coarse granular material made of waste rock. The above-mentioned aspects will be addressed in order to present a methodology for constructing an optimal numerical model that ensures stable and reliable numerical results with the minimum time of computing. The determination of model parameters is also addressed to reduce the uncertainty of numerical modeling. All the model parameters having physical meanings have been obtained by laboratory tests or by considering typical values. The only

model parameter having a clear physical meaning but remaining difficult to measure is the rolling resistance coefficient. Its value has to be obtained through a process of calibration against some experimental results obtained by repose angle tests on a waste rock. The validity and predictability of the calibrated numerical model have been successfully verified against additional experimental results.

2. Validation of the EDEM

Before conducting any numerical modeling, it is important for any new users to undergo sufficient training to know how to make use of a numerical model to produce stable and reliable numerical results. This training can be achieved through the process of numerical model validation against analytical solutions. This step, usually considered unnecessary by a large number of researchers, is crucial, especially for new users, to learn how to use the code correctly, to identify any errors or limitations in the numerical model, and to learn how to obtain an optimal numerical model that ensures stable and reliable numerical results with the shortest time of calculation [37].

In this study, the validation of the EDEM code was realized against the analytical solutions developed for calculating the normal and tangential forces at the contact between two spheres, a process similar to the works conducted by Chung and Ooi [39].

Figure 1 shows the physical model of two identical spheres moving with an initial speed of 10 m/s in opposite directions with their centers aligned in a plane parallel to their moving direction. In the figure, R is the radius of the spheres, E the Young's modulus, ρ the density, and ν the Poisson's ratio.

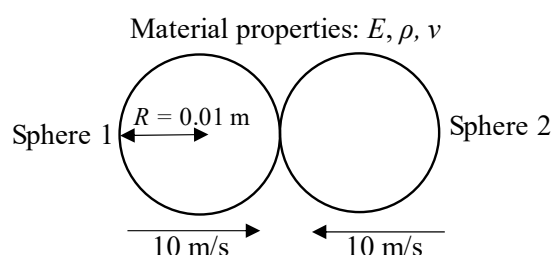


Figure 1. A physical model of two identical spheres moving with an initial speed of 10 m/s in an opposite direction with their centers aligned in a plane parallel to their moving direction.

Table 1 shows the physical and mechanical property parameters of the spheres used for the validation of the EDEM model. It needs to be noted here that the purpose of validation is to examine if the numerical model can produce the same results as the analytical solution, as long as the numerical model and analytical solution use the same given parameters values. The parameter values used for validation can thus be arbitrary and even fictive. The Hertz–Mindlin contact model is used in all the simulations of this study.

Table 1. Physical parameters of two identical spheres having a radius of 0.01 m collided with an initial speed of 10 m/s in an opposite direction.

Material of Particles	Young's Modulus, E (Pa)	Density, ρ (kg/m ³)	Poisson's Ratio, ν
Material 1	2.0×10^{11}	7750	0.3
Material 2	4.8×10^{10}	2800	0.2
Material 3	2.0×10^{10}	2500	0.25

An analytical solution for calculating the normal contact force between two spheres, F_n , has been given as follows [40,41]:

$$F_n = \frac{4}{3} \delta_n^{\frac{3}{2}} \frac{E_1 E_2}{E_2 (1 - \nu_1^2) + E_1 (1 - \nu_2^2)} \sqrt{\frac{R_1 R_2}{R_1 + R_2}} \quad (1)$$

where δ_n is the overlap of normal contact; E_1 and E_2 are the Young's moduli of sphere 1 and sphere 2, respectively; ν_1 and ν_2 are the Poisson's ratios of sphere 1 and sphere 2, respectively; and R_1 and R_2 are the radii of sphere 1 and sphere 2, respectively.

As a special case with two identical spheres having $E = E_1 = E_2$, $\nu = \nu_1 = \nu_2$, and $R = R_1 = R_2$, Equation (1) is reduced to:

$$F_n = \frac{\sqrt{2R}}{3} \delta_n^{\frac{3}{2}} \frac{E}{1 - \nu^2} \quad (2)$$

Figure 2 presents a numerical model of the EDEM to reproduce the physical model presented in Figure 1 along with the material parameters given in Table 1. As the problem does not contain any uncertainty in terms of geometrical (radius) and material properties (density, Young's modulus, and Poisson's ratio) for both physical and numerical models, a perfect agreement between numerical and analytical solutions can be expected as long as the numerical results are stable and reliable. This requires sensitivity analyses of model parameters in order to obtain an optimal numerical model that ensures stable and reliable numerical results with shortest time of computing.

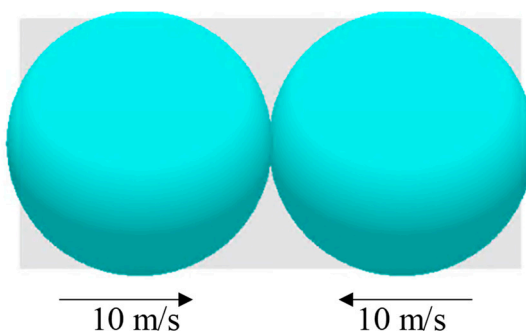


Figure 2. Numerical model of the physical model presented in Figure 1, built with the EDEM by considering the parameters given in Table 1.

For this simple problem with two spheres, the only need for the optimization of the numerical model is to perform sensitivity analysis of the time step to find the optimal time step. On the one hand, the time step should be as large as possible to shorten the time of computing. On the other hand, the stability and reliability of numerical results cannot be guaranteed if the time step is not small enough. The optimal time step corresponds to the largest time step that can ensure stable and reliable numerical results with the shortest time of computation.

Figure 3 presents the variation in the normal contact force F_n (Figure 3a) and normal contact overlap δ_n (Figure 3b) of the spheres as a function of the time step for the three cases presented in Table 1. For spheres with material 1, the numerical results (both normal contact force and normal overlap) become stable when the time step is smaller than 1.08×10^{-7} s. A further reduction in the time step does not lead to any change in the numerical results. The optimal time step for material 1 is thus determined as 1.08×10^{-7} s. Similarly, for the cases of materials 2 and 3, the optimal time steps are determined as 1.29×10^{-7} and 1.91×10^{-7} s, respectively. It is noted that the optimal time step changes as the sphere material changes. Sensitivity analysis of time step is thus necessary, case by case, to ensure stable and reliable numerical results with the shortest time of calculations.

Figure 4 presents the variation in the normal contact force F_n as a function of the normal contact overlap δ_n , both obtained by numerical modeling with the optimal time step. In the figure, the variation in the normal contact force F_n predicted by applying the analytical solution (Equation (2)) as function of the normal contact overlap δ_n is also plotted. Perfect agreements are obtained between the analytical and numerical results for all three cases from Table 1. The validity of the EDEM model is thus verified, at least partly.

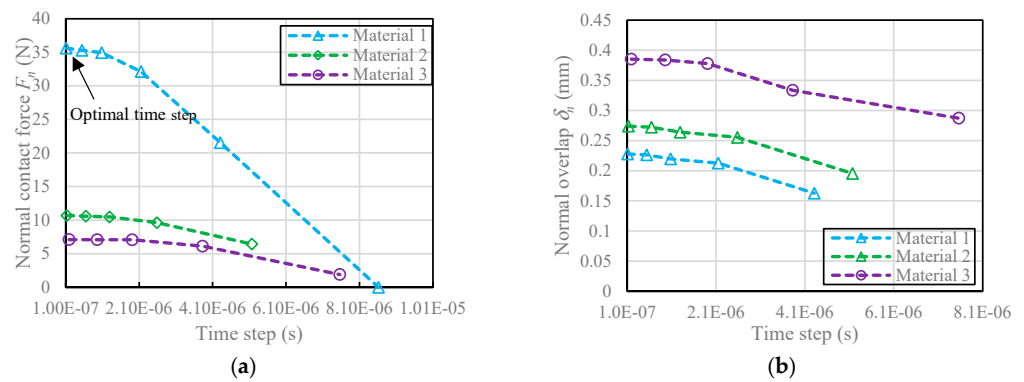


Figure 3. Variation in (a) normal contact force and (b) normal contact overlap as functions of the time step for the case of spheres with different materials.

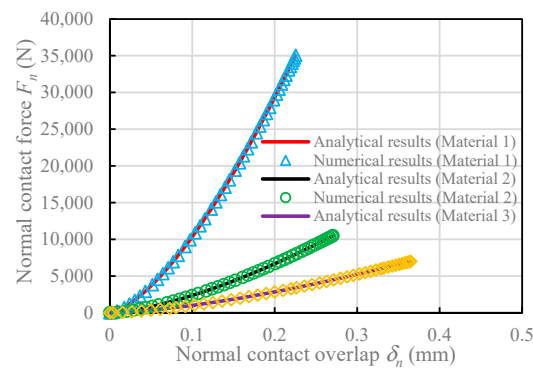


Figure 4. Variation in normal contact force F_n as function of normal contact overlap δ_n , both obtained by numerical modeling with the optimal time step and predicted by applying the analytical solution (Equation (2)).

Figure 5 presents another physical model with two identical spheres moving with an initial speed of 10 m/s in opposite directions with their centers not aligned with their movement direction. The same sphere geometries and material properties presented in Table 1 are used here.

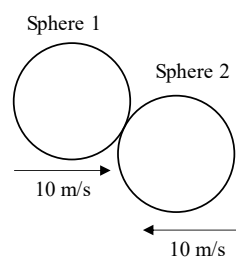


Figure 5. Physical model of two identical spheres moving with an initial speed of 10 m/s in opposite directions with their centers not aligned with their movement direction.

The analytical solution for calculating the tangential force at the contact between the two spheres, F_t , can be expressed as follows [42,43]:

$$F_t = -S_t \delta_t \quad (3)$$

where δ_t is the tangential overlap; S_t is the tangential stiffness expressed as

$$S_t = \frac{8G_1G_2}{G_2(2-\nu_1) + G_1(2-\nu_2)} \sqrt{\frac{R_1R_2}{R_1+R_2}} \delta_n \quad (4)$$

where G_1 and G_2 are the shear moduli of sphere 1 and sphere 2, respectively. As a special case with two identical spheres having $G = G_1 = G_2$, $\nu = \nu_1 = \nu_2$, and $R = R_1 = R_2$, Equation (4) is reduced to

$$S_t = \frac{2G}{2 - \nu} \sqrt{2R\delta_n} \quad (5)$$

where G is expressed as follows:

$$G = \frac{E}{2(1 + \nu)} \quad (6)$$

Figure 6 shows a numerical model of the physical model presented in Figure 5, built with the EDEM by considering the parameters provided in Table 1.

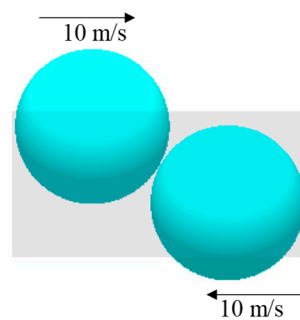


Figure 6. Numerical model of the physical model presented in Figure 5, built with the EDEM by considering the parameters provided in Table 1.

Sensitivity analyses of the time step lead to optimal time steps of 1.08×10^{-7} , 1.29×10^{-7} , and 1.91×10^{-7} s for the cases of materials 1, 2, and 3, respectively. Figure 7 presents the variation in the tangential contact force F_t as a function of the tangential contact overlap δ_t , both obtained by numerical modeling with the optimal time step. The tangential contact force F_t as a function of tangential contact overlap δ_t , predicted by applying the analytical solution (Equation (5)), is also plotted in the figure. The perfect agreement between the numerical and analytical results indicates once again that the EDEM model is validated against analytical solutions

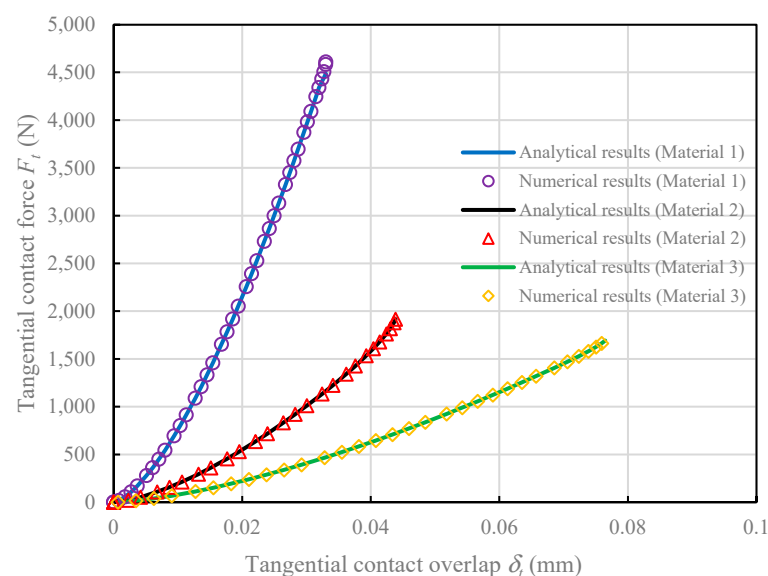


Figure 7. Variation in the tangential contact force F_t as a function of the tangential contact overlap δ_t , both obtained by the numerical modeling with the optimal time step and predicted by applying the analytical solution (Equation (5)).

3. Application of the EDEM Code for Simulating the Mechanical Behavior of Granular Material

In the previous section, the validity of the EDEM code was verified against analytical solutions. In this section, the power or applicability of the numerical model will be tested through the numerical reproduction of experimental results.

In this study, two series of tests are performed with waste rock taken from a mine located in the northwest of Québec, Canada. The test results will be reproduced by numerical modeling with the EDEM code. The experimental results obtained by the first series of tests will be used to calibrate the rolling resistance coefficient of waste rock particles, an unmeasurable model parameter. The experimental results obtained by the second series of tests are then used to test the predictability of the calibrated numerical model.

Figure 8 presents the PSD curve of the tested waste rock in terms of accumulated percentage by mass (Figure 8a) and percentage by particle number (Figure 8b) after excluding oversized and undersized particles in order for the particle sizes to be in the range of 0.315 to 8.0 mm. Figure 8b shows the variation in the percentage of particle numbers as a function of particle size in the form of a histogram. It can be fitted to a Gaussian curve by applying the normal distribution function [44]:

$$f(d) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(d - \mu)^2}{2\sigma^2}\right] \quad (7)$$

where $f(d)$ is the probability function of particle diameter, d ; μ is the mean diameter of particles; and σ is the standard deviation.

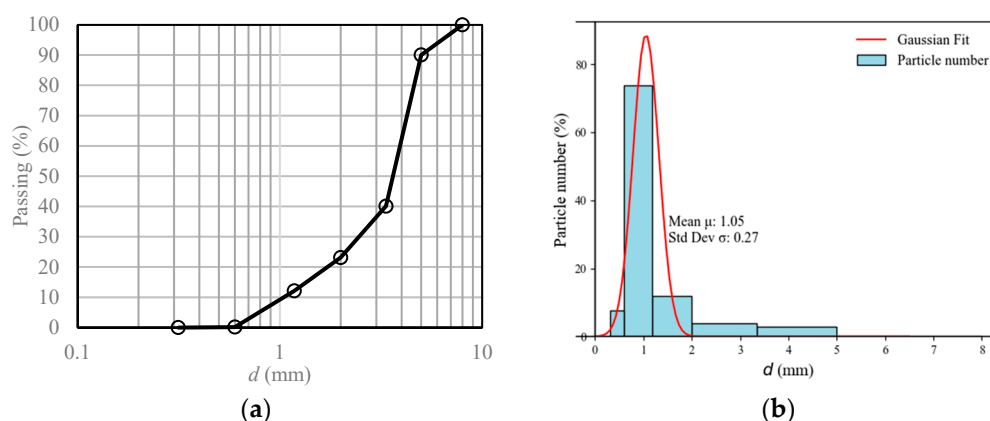


Figure 8. PSD curves of the tested waste rock in terms of (a) accumulated percentage by mass and (b) percentage by particle number.

The first series of tests was conducted to obtain the repose angle of the tested waste rock. Figure 9 shows a schematic presentation (Figure 9a) and pictures (Figure 9b) of waste rock repose angle tests. The tests were performed with a total mass of 300.5 g of waste rock, placed in a funnel having an open diameter of 19 cm on top, an open diameter of 4.0 cm at the base, and an overall height of 12 cm (Figure 9a). The tests were realized by gently (around 0.01 m/s) lifting the funnel in the vertical direction until empty, resulting in the formation of a waste rock pile on the table (Figure 9b). The height H and the diameter D of the waste rock pile were measured, respectively. The repose angle could then be calculated. The test was repeated five times, and an average repose angle θ of 36.41° was obtained for the tested waste rock.

Table 2 presents the material parameters necessary for the EDEM model. Once again, the parameters that have clear physical meanings need be determined or estimated by conducting experimental tests instead of being considered arbitrary parameters obtained by the calibration process. In Table 2, the particle density of tested waste rock was measured in our laboratory. The Young's modulus, Poisson's ratio, and static friction coefficient of the

tested waste rock were measured by Major and Knupp [45]. The restitution coefficient of tested waste rock was determined by the drop test results conducted by Sandeep et al. [46]. The rolling resistance coefficient of waste rock is unknown. This parameter is used to consider the shape effects of the non-spherical waste rock particle and has to be calibrated against the experimental results. The calibration of the rolling resistance coefficient will be introduced after.

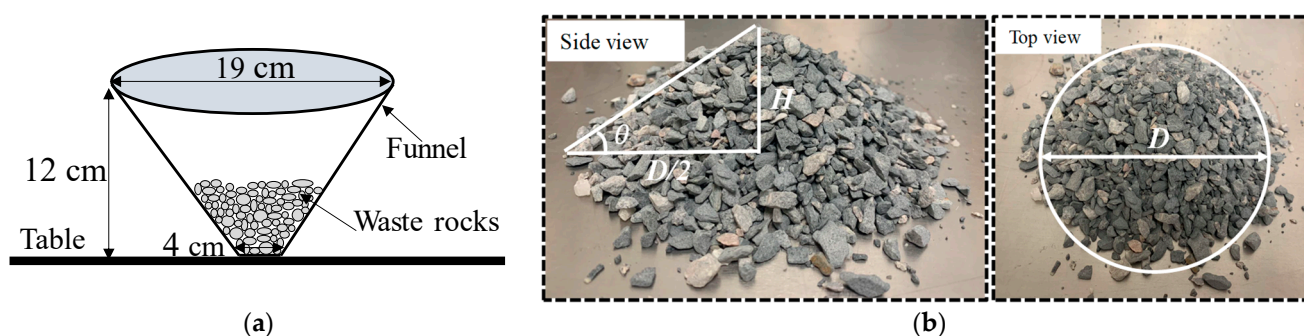


Figure 9. Waste rock repose angle test: (a) schematic presentation; (b) pictures of a repose angle test.

Table 2. Model and material parameters necessary for the EDEM model.

Material of Particles	Model and Material Parameter	Values	Determination
Waste rock particle parameters	Particle density, ρ (kg/m ³)	2760	Measured
	Young's modulus, E (GPa)	46.8	Measured ¹
	Poisson's ratio, ν	0.19	Measured ¹
Particle–particle interaction	Restitution coefficient, μ_e	0.79	Measured ²
	Static friction coefficient, μ_s	0.466	Measured ¹
	Rolling resistance coefficient, μ_r	--	Unknown

¹ measured by Major and Knupp [45] for the same waste rock; ² measured by Sandeep et al. [46].

To numerically reproduce these experimental results, the first task is to generate waste rock particles that have a PSD the same as that of the tested waste rock shown in Figure 8 in terms of percentage by mass (Figure 8a) and percentage by particle number (Figure 8b). It is possible in this study because the tested waste rock was obtained by intentionally excluding the oversized (large) and undersized (small) particles. For most cases, it is impossible to generate particles having the full PSD curve of the studied material because the fine particles can be small in percentage by mass but huge in percentage by particle number. A PSD cut must be performed to exclude a portion of fine particles by assuming that the excluded fine particles do not have any effects on the mechanical behavior of the granular materials. However, its validity needs to be verified. In this study, a good example of PSD cut will be shown through sensitivity analyses of the PSD cut to ensure stable and reliable numerical results.

Figure 10 presents five possible cuts of the PSD of the tested waste rock: PSD 1, PSD 2, PSD 3, PSD 4, and PSD 5, with particle sizes ranging from 5.0 to 8.0 mm, 3.35 to 8.0 mm, 2.0 to 8.0 mm, 1.18 to 8.0 mm, and 0.315 to 8.00 mm, respectively. PSD 5 is the same as the PSD of the tested waste rock with particle sizes ranging from 0.315 to 8.0 mm.

To generate particles with PSD 1 in the EDEM model, one should note that the particles of PSD 1 have sizes varying between 5 and 8 mm. To generate particles having sizes intermediate between 5 and 8 mm in EDEM, the Gaussian distribution with $\sigma/\mu = 0.25$ obtained from the full PSD of the tested waste rock is used. The same procedure was applied in the generation of particles of two consecutive sieves for PSD 2 to 5. Figure 11 presents the number-weighted PSD generated by the EDEM for PSD 1 to 5 using a Gaussian distribution. The generated particle numbers are 727, 2578, 5571, 14,438, and 44,415 for PSD 1, PSD 2, PSD 3, PSD 4, and PSD 5, respectively. One notes that the particle number significantly increases as smaller fine particles are taken into account.

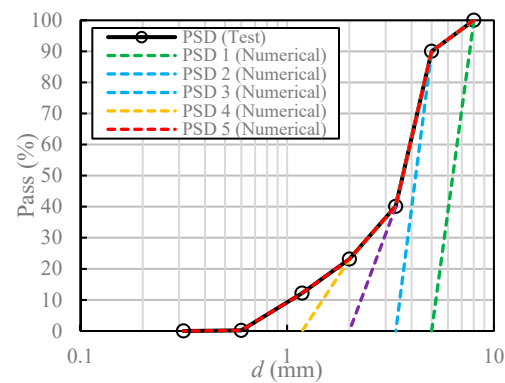


Figure 10. Different cuts of the PSD curves of the tested waste rock used in the numerical model.

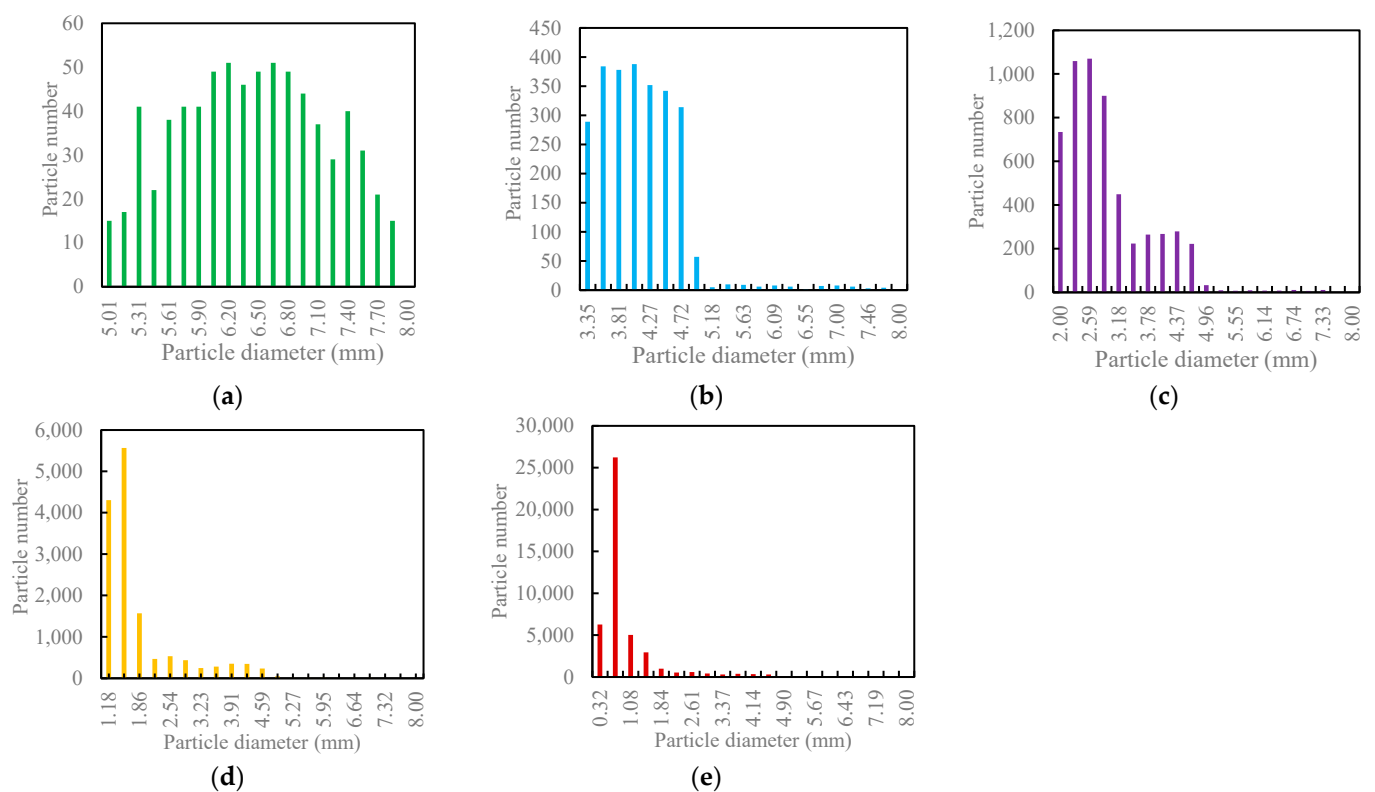


Figure 11. Particle number-weighted PSD generated by the EDEM to reproduce the different cuts of the PSD of the tested waste rock: (a) PSD 1; (b) PSD 2; (c) PSD 3; (d) PSD 4; (e) PSD 5.

Figure 12 presents the numerical models of the waste rock particles generated by the EDEM for different cuts of the PSD. The geometry of the numerical models is the same as the physical model shown in Figure 9a. The material and model parameters necessary for the EDEM model have been provided in Table 2. Spherical particles were used in the simulations to represent the non-spherical waste rocks particles. The unmeasurable angularity of particles will be reflected by the calibration of the rolling resistance coefficient. In the figure, the numerical model with the waste rock particles generated by the EDEM for the full PSD curve (PSD 5) is also plotted. One sees clearly that the particle distributions generated by applying the PSD cut become closer to that generated by applying the full PSD curve of the tested waste rock as the excluded fine particle size decreases.

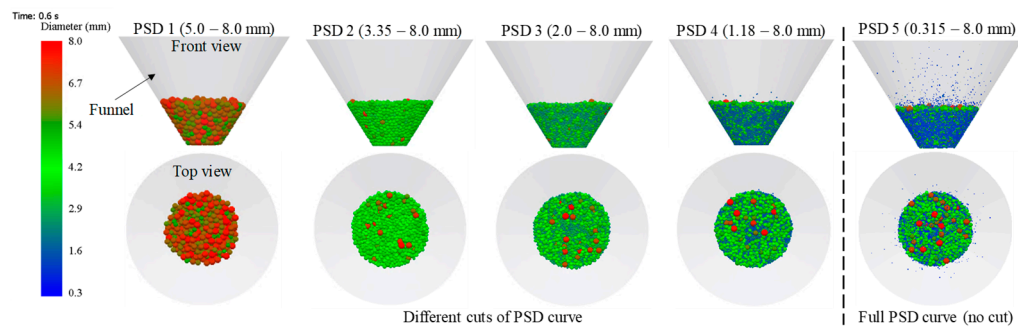


Figure 12. Numerical models with the waste rock particles generated by the EDEM by applying four different PSD cuts and the full PSD of the tested waste rock.

Once the waste rock particles are generated in the EDEM model, the flow of particles can be simulated. Figure 13 shows the states of the particles generated by the EDEM for the case of PSD 1 from the beginning to the end of the repose angle test. The waste rock particles were first generated in the funnel by using the dynamic factory of the EDEM with a generation rate of 2 kg/s (Figure 13a). After that, the funnel was lifted up with a speed of 0.01 m/s in the vertical direction. Figure 13b shows the formation of a waste rock pile on the table at an intermediate stage. Figure 13c shows the state of the waste rock pile at the end of numerical simulation. The repose angle θ of the waste rock pile was obtained by using the protractor tool in the EDEM by clipping the waste rock pile in the center.

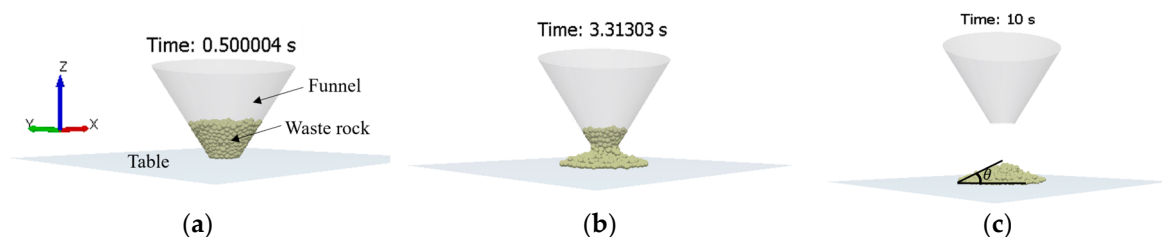


Figure 13. Numerical model built with the EDEM for case of PSD 1: (a) initial state; (b) intermediate state; (c) final state.

The same numerical modeling process for PSD 1 were repeated for the cases of PSD 2 to 5. In all the cases, time step sensitivity analyses were performed first to ensure stable and reliable numerical results. Figure 14 presents the variations in the repose angle of the waste rock pile as a function of the time step, obtained by numerical modeling with the EDEM for PSD 1 to 5 using a rolling resistance coefficient of 0.05. For all the cases, the numerical modeling results in a repose angle of 0° when a large time step is used, meaning that all the particles were lost in the numerical simulation due to the overly large time step. For PSD 1, the numerical results become stable when the time step is equal to or smaller than 3.24×10^{-6} s. The optimal time step is thus determined as 3.24×10^{-6} s. Similarly, the optimal time steps are determined as 2.17×10^{-6} , 1.29×10^{-6} , 3.83×10^{-7} , and 1.02×10^{-7} s for PSD 2, PSD 3, PSD 4, and PSD 5, respectively. One notes that the optimal time step decreases as the content of fine particles increases. In addition, one notes that the repose angles obtained by the EDEM model by using a rolling resistance coefficient of 0.05 are much smaller than the measured value of $\theta = 36.41^\circ$.

Figure 15 presents the variation in the repose angle of the waste rock pile as a function of the PSD cut, obtained by numerical simulations with the optimal time steps for three different rolling resistance coefficients μ_r . One notes that the repose angle of the waste rock increases as the content of fine particles increases from PSD 1 to PSD 3. The repose angle becomes stable (constant) at PSD 3, indicating that including more and smaller fine particles does not have any effect on the repose angle of the tested waste rock. The repose angle of the tested waste rock with a full curve of PSD 5 (0.315–8.0 mm) can be obtained

by using the curve of PSD 3 (2.0–8.0 mm) in the numerical model. The optimal cut of PSD thus corresponds to PSD 3 (2.0–8.0 mm).

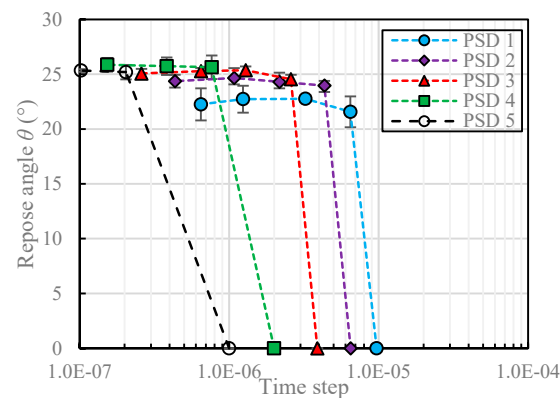


Figure 14. Variation in the repose angle as a function of the time step, obtained by numerical simulations with the parameters shown in Table 2 and a rolling resistance coefficient of 0.05 for five different cuts of PSD.

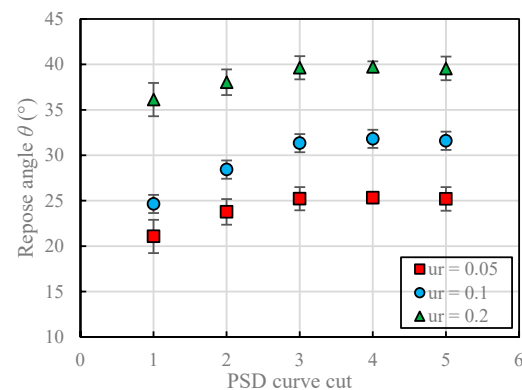


Figure 15. Variation in the repose angles of waste rock piles as a function of the PSD cut, obtained using numerical simulations with the parameters shown in Table 2 along with the optimal time steps for three different rolling resistance coefficients μ_r .

Figure 16a presents the variations in the repose angle of the waste rock with the optimal cut of PSD 3 (2.0–8.0 mm) as a function of the time step, obtained by numerical modeling with different values for the Young's modulus of the tested waste rock. The value of 4.68×10^{10} Pa corresponds to the measured value shown in Table 2, while 4.68×10^3 Pa is obtained by reducing the measured Young's modulus by a factor of 10^7 . The other input parameters for the EDEM numerical model are given in Table 2 along with a rolling resistance coefficient of 0.05. The optimal time steps are determined as 6.48×10^{-7} , 6.48×10^{-6} , 7.0×10^{-6} , 1.30×10^{-5} , 4.10×10^{-5} , and 6.48×10^{-5} s for Young's moduli of 4.68×10^{10} , 4.68×10^8 , 4.68×10^7 , 4.68×10^6 , 4.68×10^5 , and 4.68×10^4 Pa, respectively. The results indicate that the optimal time step decreases as the Young's modulus of waste rock particles increases. This can be explained as follows from the dynamic physics of particle–particle and particle–ground surface interactions.

For particles having large Young's modulus values, the particles are harder. The jumping and inter-hitting of particles can be faster and stronger. A long time is necessary to allow the system to settle down and reach a static equilibrium. But a short time step is necessary to capture the intermediate responses of particles movement. When one attributes a much smaller value to the waste rock particles, the particles become much softer than those of the actual material. The jumping and inter-hitting of particles become much slower and weaker. A static equilibrium can be achieved quickly. This explains why the optimal time step becomes longer. More interestingly, this explains well why the time of calculation

can be shortened through a reduction in the Young's modulus. Strictly said, however, the use of a smaller Young's modulus than the actual value of waste rock particles means the simulation of another physical model, no longer the original one, even though the obtained repose angle can be very close to that obtained by using the actual Young's modulus as long as the Young's modulus is not reduced to a value smaller than 4.68×10^7 Pa. Beyond that value, the EDEM model can lead to an underestimate of the repose angle, as shown in Figure 16b. The optimal Young's modulus for this mechanical problem can thus be determined as 4.68×10^7 Pa. Numerical modeling with any values smaller than this optimal Young's modulus cannot guarantee stable and reliable numerical results.

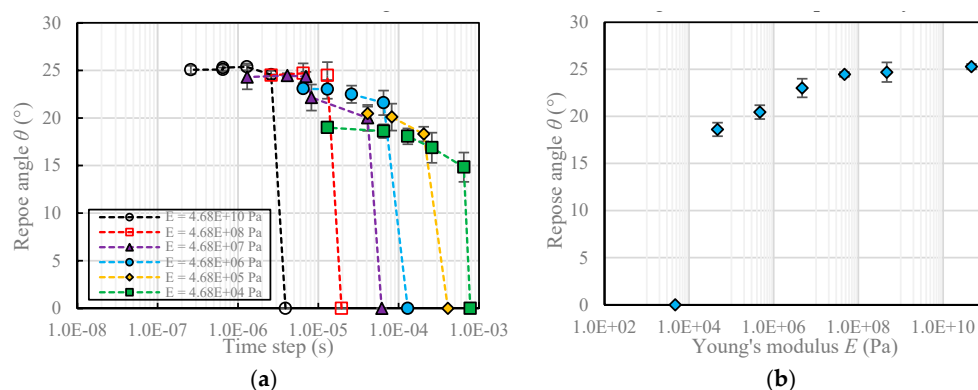


Figure 16. (a) Variations in repose angle as a function of the time step, obtained by numerical modeling by using the optimal cut of PSD 3 and a rolling resistance coefficient of 0.05 for different Young's moduli; (b) variation in the repose angle as a function of the Young's modulus using the optimal time step.

These results and analysis indicate that it is indeed advantageous to use a reduced value for Young's modulus to accelerate the numerical calculations for some specific mechanical problems. Nevertheless, the Young's modulus of granular materials should not be decreased in an arbitrary way. Otherwise, the stability and reliability of the numerical results cannot be guaranteed. Similar findings have been reported by Lommen et al. [47].

Figure 17 shows the variation in the repose angle of waste rock piles as a function of the rolling resistance coefficients μ_r obtained by numerical simulations with the optimal numerical model (i.e., with the optimal cut of PSD 3 (2.0–8.0 mm), optimal Young's modulus of 4.68×10^7 Pa, and optimal time step of 4.10×10^{-6} s), determined by several sensitivity analyses. The measured repose angle of $\theta = 36.41^\circ$ for the tested waste rock is also plotted in the figure. One sees that the best agreement between the numerical and experimental results can be obtained by using a rolling resistance coefficient of $\mu_r = 0.16$.

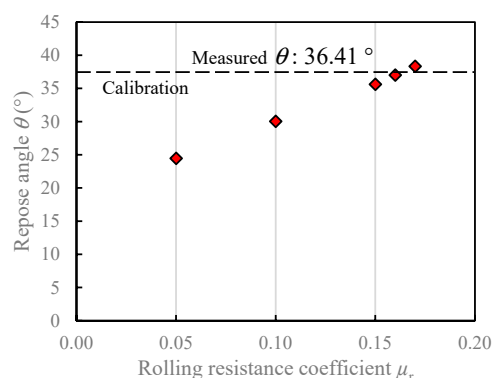


Figure 17. Variation in repose angle as a function of rolling resistance coefficients μ_r , obtained by numerical simulations with the optimal numerical model (i.e., with the optimal time step of 4.10×10^{-6} s, optimal Young's modulus of 4.68×10^7 Pa, and optimal cut of PSD 3).

The material parameters given in Table 2 and the EDEM model along with the optimal cut of PSD 3 (2.0–8.0 mm), optimal Young's modulus of 4.68×10^7 Pa, and rolling resistance coefficient of $\mu_r = 0.16$ constitute the calibrated numerical model, which can be applied to predict the mechanical behavior of the tested waste rock in different testing conditions. Its validity and predictability will be verified against another series of tests realized to evaluate the effect of the falling height H_F of waste rock on the repose angle of the tested waste rock.

Figure 18 shows a schematic presentation of the tests. A total mass of 300.5 g of waste rock was placed in the same funnel as the one used in the first series of tests. The waste rock was then dropped on the table at a falling height of H_F . Figure 19 presents the side and top views of the waste rock piles generated by dropping the waste rock from three different falling heights. It can be seen that the repose angle θ decreases from 27.9° to 21.2° , while the diameter D of the waste rock piles increases from 14.5 to 15.5 cm as the falling height increases from 6 to 15.5 cm.

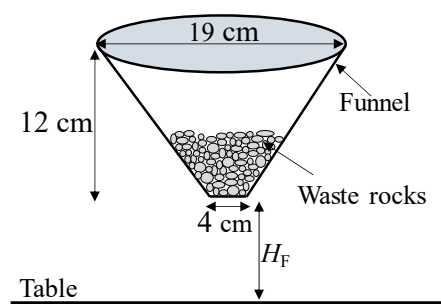


Figure 18. Schematic presentation of waste rock dropped at a falling height of H_F .

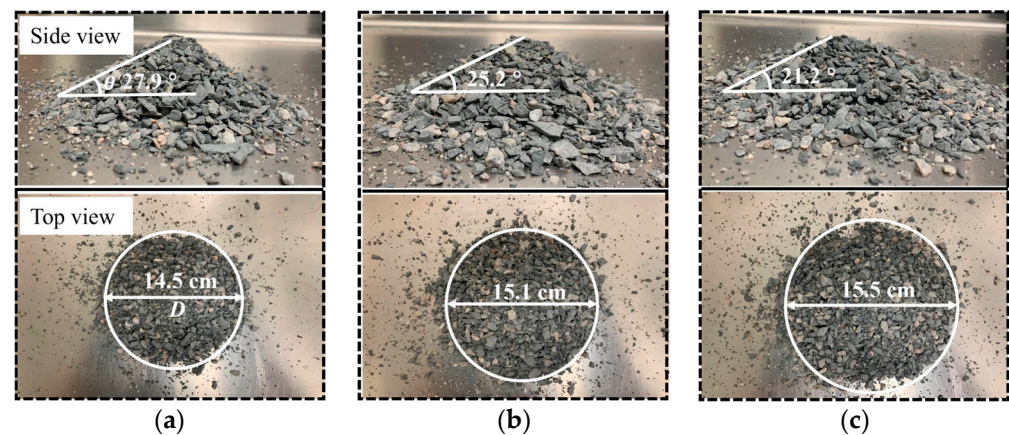


Figure 19. Side and top views of waste rock piles generated by dropping waste rock from different falling heights: (a) $H_F = 6$ cm; (b) $H_F = 10.5$ cm; (c) $H_F = 15.5$ cm.

Figure 20 presents the calibrated numerical model with the material parameters given in Table 2, rolling resistance coefficient $\mu_r = 0.16$, optimal Young's modulus of 4.68×10^7 Pa, optimal time step of 4.10×10^{-6} s, and optimal cut of PSD 3 (2.0–8.0 mm) to predict the effects of falling height H_F on the repose angle of the tested waste rock. The geometry of the numerical model is the same as that of the physical model shown in Figure 18. In the simulations, waste rock particles were generated first in the funnel. The bottom was blocked with a plate attached to the bottom (Figure 20a). The vertical distance between the funnel bottom and the table is equal to the falling height of H_F . The plate was removed at the end of the generation of all the particles (Figure 20b). A waste rock pile was generated on the table once all the waste rock particles were dropped on the table (Figure 20c). The total simulation time was set to be 10 s.

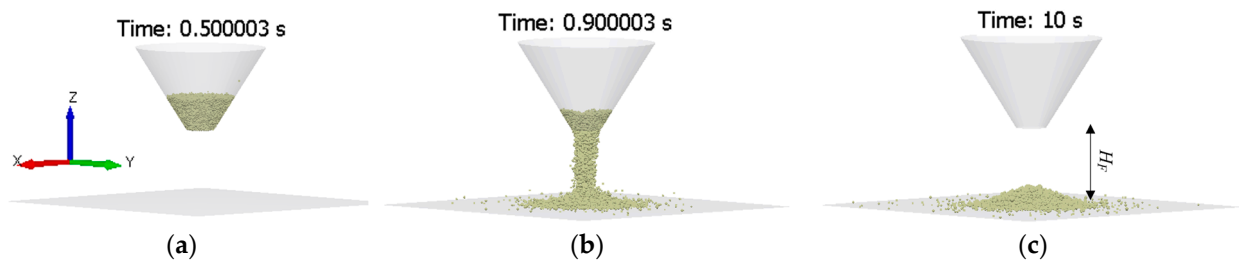


Figure 20. Calibrated numerical model (with the material parameters given in Table 2, rolling resistance coefficient $\mu_r = 0.16$, optimal Young's modulus of 4.68×10^7 Pa, optimal time step of 4.10×10^{-6} s, and optimal cut of PSD 3) for predicting the effects of falling height H_F on the repose angle of waste rock: (a) initial state; (b) intermediate state; (c) final state.

Figure 21 presents the side views (Figure 21a) and top views (Figure 21b) of waste rock piles, obtained by numerical modeling with the calibrated numerical model for different falling heights. The repose angle θ (Figure 21a) and the diameter D (Figure 21b) of the waste rock piles were estimated by using the protractor tool and ruler tool in the EDEM, respectively.

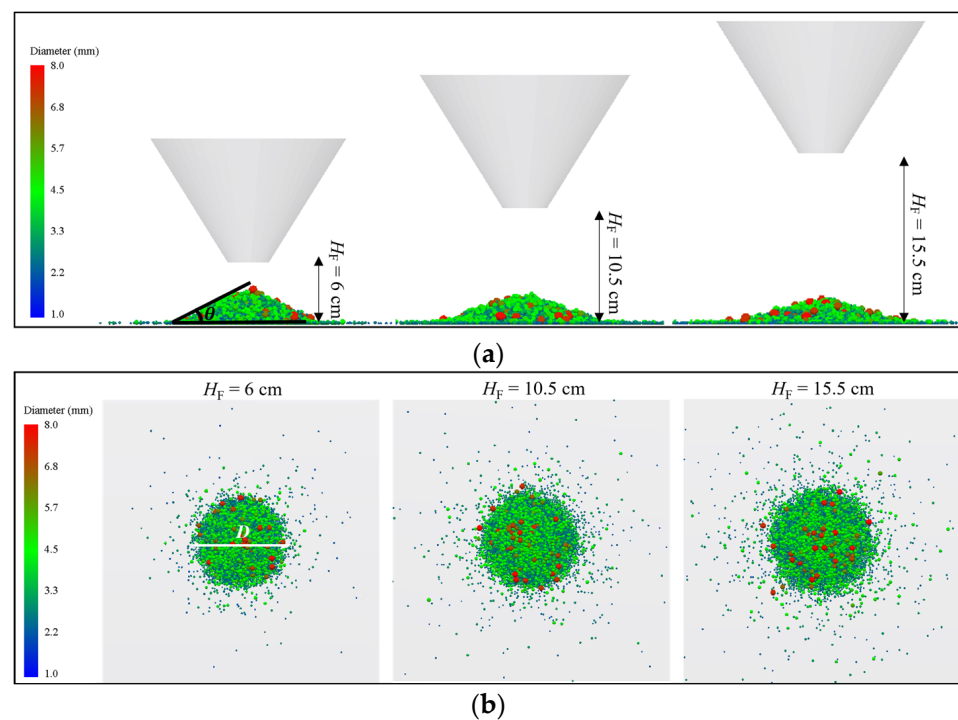


Figure 21. Views of waste rock piles with different falling heights H_F obtained by the calibrated numerical model: (a) side views; (b) top views.

Figure 22 presents the repose angles θ (Figure 22a) and diameters D (Figure 22b) of waste rock piles as functions of the falling height H_F , obtained by laboratory tests and predicted by numerical modeling with the calibrated model. Good agreements are obtained between the experimental results and numerical predictions for both the repose angles and the diameters of waste rock piles for all the three different falling heights. These results indicate that the validity and predictability of the calibrated numerical model to simulate the mechanical behavior of granular materials have been successfully verified. It can be used to analyze the mechanical behavior of structures made of the tested waste rock under different conditions.

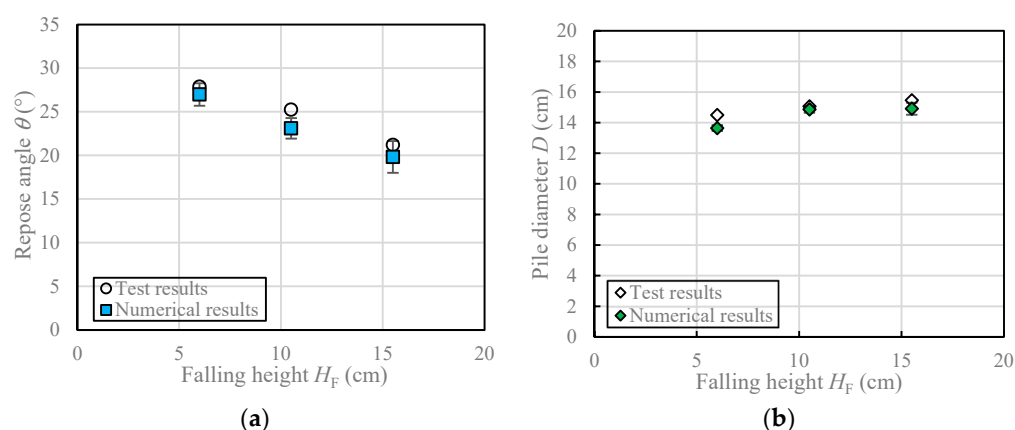


Figure 22. Variations in the (a) repose angle θ and (b) pile diameter D as functions of the falling height H_F , obtained by laboratory tests and predicted by the calibrated numerical model.

4. Discussion

In this study, we have shown how to obtain an optimal numerical model with an optimal cut of the PSD curve, an optimal time step, and an optimal Young's modulus to ensure stable and reliable numerical results with the shortest calculation time. The validity of the EDEM numerical model has been verified against the analytical solution, while the applicability of the numerical model has been confirmed by the numerical reproduction and prediction of experimental results. The methodology can be applied to any other numerical codes based on the discrete element method for mechanical behavior analyses. Nevertheless, it should be kept in mind that the methodology also has certain limitations.

In the study, spherical particles were used in the EDEM simulation to represent the non-spherical waste rock particles. The shape effect of waste rock particles was accounted for by calibrating the rolling resistance coefficient against the results of waste rock repose angle tests. However, the spherical particles may not fully capture the behavior of waste rock, where the particle shape has a significant influence. Future studies should incorporate the actual shape of waste rock particles for simulations that are closer to reality.

Laboratory sieving analysis can determine the mass proportion of particles with standard sieve sizes. However, the actual particle size distributions (e.g., particle sizes and corresponding mass proportions) between two consecutive standard sieves are unknown due to the lack of intermediate sieves. Assumptions and approximations, such as the Gaussian distribution used in this study, have to be made in the numerical model to generate particles between the two neighboring sieves. Therefore, the PSD generated by the EDEM may not fully correspond to the actual PSD of the tested waste rocks between the two consecutive sieves. More research is necessary to obtain more representative particle distribution between two neighboring sieves.

In this study, the Young's modulus of waste rock was artificially reduced in the numerical model to reduce the DEM simulation time. The numerical results did not significantly change when the Young's modulus was larger than the optimal Young's modulus determined by sensitivity analyses. These findings suggest that reducing the Young's modulus can be used in the DEM simulations for determining the repose angle of waste rock. However, it is unknown if this approach still applies to determining other behaviors of waste rock. It is generally recommended that the physical parameters of materials should not be altered in the numerical model, as these changes mean changes in the physical problem that does not correspond to the modeled problem.

This study aims to demonstrate how to achieve an optimal (particle size distribution) PSD cut by excluding fine particles. The methodology is only considered valid for mechanical behaviors (e.g., repose angle) because fine particles, where their sizes and quantities are negligible compared to the pores or void spaces created by larger particles, can remain free within these spaces. This justifies performing PSD cuts by excluding some

fine particles through sensitivity analysis. However, this methodology is not applicable for simulating the hydraulic and thermal behavior of granular materials, as these properties are significantly influenced by the sizes and quantities of fine particles. Additionally, it cannot be used in simulations where fine particles contribute to cohesive forces. For such analyses, a new methodology is required.

The total mass of waste rock used in this study was 300.5 g, with a maximum particle size of 8.0 mm. The mass and maximum particle size of the waste rock are considerably smaller than those typically found in field conditions. The impact of waste rock particle size and mass on the repose angle of waste rock will be investigated in future studies.

The proposed general methodology (for obtaining an optimal numerical model through diverse sensitivity analyses) can be used to obtain optimal numerical models for any other granular materials. However, additional studies may be necessary to further confirm its effectiveness for a wider range of granular materials.

5. Conclusions

This study proposes a methodology for constructing an optimal DEM numerical model to obtain stable and reliable numerical results of mechanical behaviors of granular materials with the shortest time of computing. The validation of the numerical model against the analytical solution is emphasized for new users. An optimal numerical model with an optimal PSD cut, optimal time step, and optimal Young's modulus can be obtained by conducting sensitivity analyses. Calibration is only recommended for model parameters that cannot be measured or if their measurements are not reliable. The numerical model, along with the material parameters and the calibrated model parameters, constitute a calibrated numerical model. The validity and predictability of the calibrated numerical model needs to be tested against additional experimental results. More conclusions and suggestions are summarized as follows:

- The good agreements between the numerical and analytical results for the normal contact force and tangential contact force between two spheres indicate the EDEM code is validated.
- To simulate the mechanical behavior of granular materials, a portion of fine particles can indeed be neglected to reduce the simulation time. However, the PSD cut for excluding fine particles cannot be performed arbitrarily. Sensitivity analyses of the PSD cut must be performed to obtain the optimal cut of the PSD curve, ensuring stable and reliable numerical results.
- The Young's modulus of granular materials can be diminished to reduce the required time step and accelerate the achievement of a static equilibrium state as long as the Young's modulus is larger than a critical value. The optimal Young's modulus should be determined by performing a sensitivity analysis to ensure stable and reliable numerical results with the shortest time of calculations. The physics and mechanism have been for the first time explained. The use of a value for the Young's modulus smaller than the actual value of waste rock particles causes the simulation of another physical model, no longer the original one, even though the obtained repose angle can be very close to that obtained by using the actual Young's modulus.
- Sensitivity analyses of the time step need to be performed case by case to find the optimal time step that ensures stable and reliable numerical results with the minimum time of calculation.
- In numerical modeling, physical and mechanical parameters should be measured for as long as possible. The measured values should be directly used to reduce the number of model parameters obtained through calibration. They should not be simply neglected, changed, or calibrated unless their measurements are unreliable with valid justifications.
- The good agreements between the experimental results and numerical predictions indicate that the calibrated DEM model can be used to simulate the mechanical behavior of granular materials.

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