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The angle of repose and size segregation of iron ore granules: DEM analysis and experimental investigation

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Abstract

We have developed a DEM model to study the packing characteristics of iron ore granules. Two important indices in characterising the packing of granules, i.e. the angle of repose (for packing stability) and a size segregation index, were obtained from the simulations. The comparisons of the simulated and experimental angle of repose and size segregation indices showed good agreement, demonstrating that the developed model is capable of predicting the behaviour of iron ore granules during pile formation. The simulation results show that the angle of repose of iron ore granules was greatly influenced by sliding and rolling friction coefficients. The simulation results showed that the decrease in granule size significantly increased the kinetic energy dissipation rate of the discharged granules during the packing process. Therefore, an increase in granule pile stability was observed. The simulation results also demonstrated the presence of significant size segregation of iron ore granules in the pile in the horizontal direction. The average granule size in the outer section of the pile was relatively larger than that in the central section. However, in the vertical direction, due to the interaction of multiple segregation mechanisms, size segregation was not clearly observed.

Keywords: Granule packing; Discrete element method; Iron ore granules; Angle of repose; Size segregation

1. Introduction

The study of granular materials is of great importance in engineering sciences due to the ever-increasing requirement of understanding granular material behaviour in both natural phenomena and industrial processes. Although a vast array of breakthroughs has been made in this area, compared to the studies on other materials like solids and liquids, there is still no integrated and generally acknowledged theory of granular materials [1]. Admittedly, it is extremely difficult to fully comprehend the behaviour of granular materials as it varies significantly under different environment and experimental conditions. Therefore, due to its complexity, the best research approach at present might be to study granular material behaviour at both macro- and microscopic scales [1-3].

To understand the microscopic behaviour such as the interaction between individual particles, numerical simulation of granular materials has rapidly developed over the past decades. Discrete Element Method (DEM) [4] has made it possible to obtain bulk particle phenomena and other dynamic information from individual particle behaviour. This technique has complemented the experimental measurements carried out at the macroscopic scale, to a large extent. For instance, DEM has been widely used in a variety of theoretical granular material research topics, such as particle impact [5-7], particle packing [8-13], particle flow [14-19] and particle-fluid flow [20-23].

In the ironmaking industry, DEM simulations have also made a great contribution to the deeper understanding of many particulate processes and the solutions of several long-term technical problems

[24-28]. The relevant studies range from simulating the behaviour of iron ore granulated mix or pellets [24, 25] in a tumbling drum to modelling particle flow during a discharging process from the top bunker of a blast furnace [26-28]. However, the simulation of the packing of iron ore granules has seldom been carried out despite its importance in the ironmaking industry. For instance, in sintering processes, the packing structure of the iron ore granules packed on a sinter strand directly affects the bed permeability and thus, the sintering productivity and sinter quality [29]. To investigate the packing of iron ore granules at an industrial scale, a comprehensive model that can predict the motion of the granules under different operating conditions is required. However, realising such a model is still quite difficult at present because many factors, such as granule properties, charging configuration and operational parameters) need to be considered.

Therefore, before modelling the packing of iron ore granules on a sinter strand at an industrial scale, bench-scale simulations of granule packing in a rectangular container could be first carried out as an intermediate step. In this paper, the characterisation of the packing of iron ore granules by some important indices, such as angle of repose and size segregation, is presented. The angle of repose is an important macroscopic parameter that reflects the stability of granule packing and internal friction behaviour of granules [30]. Size segregation is another important parameter as it provides information about the level of the uneven granule size distribution within a packed bed or pile. By comparing the indices obtained from both simulations and experiments, the model established to simulate the packing of iron ore granules has been effectively validated and improved. Therefore, such a fundamental study could provide valuable information for further investigating the packing of iron ore granules on a moving strand at an industrial scale.

Studies on particle packing have been carried out by many researchers in the last decades [31-42]. For instance, Grasselli and Herrmann [31] experimentally investigated the angle of repose of sand powders and glass spheres (100~400 μm) in a turnable container. They found out that there was an exponential decay relationship between the angle of repose and the gap between the container walls. Zhou *et al.* [32] [33] numerically investigated the relationship between the angle of repose of spherical particles and primary particle properties (*e.g.* particle size and friction coefficient) by means of DEM simulation. They validated their model by carrying out the experiments of pile formation using glass beads. Rahman *et al.* [40] applied a screening layer model [43] to study the mechanism of the segregation in the flowing layer of a conical pile using a mixture of multi-sized particles. They proposed that the zone containing the segregating component around the central feeding point expanded by increasing the initial mixing ratio, the feed rate and the flow length of the pile surface. Benito *et al.* [41] experimentally studied the segregation of quasi 2D grain piles formed by dropping glass beads of two different sizes simultaneously. They analysed [41] the influence of the free fall height of particles, the size ratios and the amplitude of the injection point displacement on the level of segregation. Despite the numerous published work on the angle of repose [31-39] and size segregation [40-42], the application of their results to the packing of iron ore granules is not straight forward. The reason is that the physical and geometrical properties of the iron ore granules are specific to the granulation technique used in ironmaking, so their properties are largely different from other granular materials (*e.g.* glass beads, sands and iron ore fines) [31-42]. For instance, the Young's modulus and the coefficient of restitution of iron ore granules, due to their porous outer layers, are much lower than those of glass beads or sands. The sliding and rolling friction coefficients of iron ore granules, compared to glass beads, are also generally larger due to their rougher surfaces and more irregular shapes.

To gain insight into the packing structural properties of iron ore granules, a nonlinear DEM model has been established for simulating the behaviour of iron ore granules during packing process. To accomplish the model, firstly the material properties (*e.g.* Young's modulus) and the particle

characteristics (*e.g.* size) of iron ore granules were determined based on corresponding measurement results. Secondly, the interactions between individual granules were realistically represented by appropriate force models. By referring to the methodologies described in the former researches [31-33], we carried out the packing of iron ore granules in a rectangular container. To characterise the granule packing, the angle of repose and size segregation have been studied. The simulated values of these parameters were compared to their experimental counterparts for model validation.

2. DEM Methodology

2.1 Governing equations and force models

DEM modelling is based on the idea that bulk particle behaviour emerges from the accurate quantification of the interparticle contact forces and the motion of individual particles. For a single particle i with mass m_i and moment of inertia I_i , the governing equations for its translational and rotational motion can be generally written as:

$$m_i \frac{d\mathbf{v}_i}{dt} = \sum_{j=1}^n (\mathbf{F}_{i,j}^C + \mathbf{F}_{i,j}^D) + m_i \mathbf{g} \quad (1)$$

$$I_i \frac{d\boldsymbol{\omega}_i}{dt} = \sum_{j=1}^n (\mathbf{T}_{i,j} + \mathbf{M}_{i,j}) \quad (2)$$

where $\mathbf{v}_i$ and $\boldsymbol{\omega}_i$ are the translational and angular velocities of particle i . The simulated forces include particle weight $m_i \mathbf{g}$, elastic contact force $\mathbf{F}_{i,j}^C$ and viscous contact damping force $\mathbf{F}_{i,j}^D$. $\mathbf{T}_{i,j}$ is the torque generated by tangential contact forces and it causes particle i to rotate. $\mathbf{M}_{i,j}$ is the rolling friction torque that opposes the rotation of particle i .

2.1.1 Contact force models

The elastic contact force model used in this work is non-linear Hertz-Mindlin no-slip model [44]. This model uses the elastic theory of Hertz [45] for the normal contact and the no-slip solution of the tangential contact theory proposed by Mindlin [46] for the tangential direction. The normal elastic contact force is expressed as a function of the relative normal displacement δ_n :

$$\mathbf{F}_{i,j}^{C,n} = -\frac{4}{3} E^* \sqrt{R^*} \delta_n^{\frac{3}{2}} \mathbf{n} \quad (3)$$

where E^* is the effective Young's modulus given by $1/E^* = (1-\sigma_i^2)/E_i + (1-\sigma_j^2)/E_j$ and R^* is the reduced radius given by $1/R^* = 1/R_i + 1/R_j$ of two particles or of particle and wall. $\mathbf{F}_{i,j}^{D,n}$ contributes to the energy dissipation due to the normal contact [44]:

$$\mathbf{F}_{i,j}^{D,n} = -\eta_n \left(\frac{4}{3} m^* E^* \sqrt{R^*} \delta_n^{\frac{3}{2}} \right)^{\frac{1}{2}} \mathbf{v}_{n,ij} \quad (4)$$

where m^* is the equivalent mass of two contacting bodies $1/m^* = 1/m_i + 1/m_j$, $\mathbf{v}_{n,ij}$ is the relative velocity at the contact point in the normal direction and η_n is the damping parameter related to the coefficient of restitution e [47].

In the tangential direction, according to the no-slip elastic solution proposed by Mindlin [46], the force-displacement relation is expressed as:

$$\mathbf{F}_{i,j}^{C,t} = -8G^* \sqrt{R^*} \delta_n \delta_t \mathbf{t} \quad (5)$$

where G^* is the effective shear modulus given by $1/G^* = (1-\sigma_i^2)/G_i + (1-\sigma_j^2)/G_j$ of two bodies in contact. Based on Eq. (5), Renzo and Maio [48] further improved the accuracy of this solution by adding a fractional parameter to the model:

$$\mathbf{F}_{i,j}^{C,t} = -\frac{2}{3} \left(8G^* \sqrt{R^* \delta_n^*} \delta_t \right) \mathbf{t} \quad (6)$$

This modification solved the problem of the unrealistic symmetric evolution of tangential force about the middle of the contact duration and makes the model as accurate as the intricate theory of micro-slip proposed by Mindlin and Deresiewicz [49] in most cases [48]. Therefore, Eq. (6) was adopted in the modelling to calculate the tangential elastic force of two contacting bodies. In addition, the tangential damping force $\mathbf{F}_{i,j}^{D,t}$ was calculated using a similar expression to Eq. (4):

$$\mathbf{F}_{i,j}^{D,t} = -\eta_t \left(\frac{4}{3} m^* E^* \sqrt{R^* \delta_n^*} \right)^{\frac{1}{2}} \mathbf{v}_{t,ij} \quad (7)$$

where $\mathbf{v}_{t,ij}$ is the tangential velocity at the contact point $\mathbf{v}_{t,ij} = \mathbf{v}_{ij} - \mathbf{v}_{n,ij} + R^*(\boldsymbol{\omega}_i + \boldsymbol{\omega}_j) \times \mathbf{n}$. The damping coefficient η_t in the tangential direction is assumed to be equal to η_n [44]. The resultant tangential force $\mathbf{F}_{i,j}^t$ (the sum of $\mathbf{F}_{i,j}^{C,t}$ and $\mathbf{F}_{i,j}^{D,t}$) is subjected to the Coulomb's law of friction. If the following relation is satisfied,

$$|\mathbf{F}_{i,j}^t| > \mu |\mathbf{F}_{i,j}^n| \quad (8)$$

then gross sliding would occur at the contact and the tangential force is given by

$$\mathbf{F}_{i,j}^t = -\mu |\mathbf{F}_{i,j}^n| \mathbf{t} \quad (9)$$

where μ denotes static friction coefficient and is assumed to be also valid in sliding conditions.

2.1.2 Rolling friction model

Although some strategies have been proposed [50, 51] to fulfil the modelling of irregular particles, the techniques are very computationally demanding, particularly for systems containing thousands of particles. Therefore, to reduce the complexity of contact detection and contact force calculation, so far the particle shape adopted in DEM model is still assumed to be spherical in most cases. However, to represent the effect of particle shape on the flowing behaviour [52, 53], including dissipating energy during relative rotation and providing stability during pile formation, a proper rolling friction model should be considered.

In general, the rolling friction models that are commonly used in DEM simulations, according to the review of Ai *et al.* [52], can be classified as directional constant torque model [30, 54], viscous model [55, 56] and elastic-plastic spring-dashpot model [57, 58]. In this paper, the first model was adopted to represent rolling friction because it has a simple expression and also works well in modelling pseudo-static particulate systems [52]. The expression of the rolling friction model is given by:

$$\mathbf{M}_{i,j} = -\mu_r R^* |\mathbf{F}_{i,j}^n| \frac{\boldsymbol{\omega}_{rel}}{|\boldsymbol{\omega}_{rel}|} \quad (10)$$

where $\boldsymbol{\omega}_{rel}$ denotes the relative angular velocity at the contact $\boldsymbol{\omega}_{rel} = \boldsymbol{\omega}_i - \boldsymbol{\omega}_j$.

2.2 Determination of model parameters

To determine the size distribution of the iron ore granules used in this study, a bulk sample of granules was made by mixing a typical blend of raw iron ore fines with 8.5 wt.% water in a tumbling drum (Fig. 1). Then, the sample granules were sized with 2.0 mm, 4.0 mm, 6.0 mm, 8.0 mm, 10.0 mm sieves and the resulting weight percentage of the granules in each size range were measured (see Table 1) for the following simulations. The average apparent density of the sample granules was also measured using a fluid displacement method [59].

Fig. 1 Samples of the iron ore granules (left) and laboratory-scale tumbling drum for granulation (right).

Furthermore, the average Young's modulus of the sample granules was measured using the Shimadzu Autograph universal tester shown in Fig. 2. As Fig. 2 shows, in one test an iron ore granule of a given size was placed onto the static plane of the tester and then the tester piston (Young's modulus $E = 200$ GPa, Poisson ratio $\sigma = 0.3$) started to move towards the plane at the speed of 0.01 mm/s until the granule was crushed. Finally, the test data showing the relationship between the compression force F_n and granule indentation δ_n at the compression stage was directly provided by the computer interface of the Shimadzu Autograph software. Then, the Young's modulus of the sample granule was calculated by the data points of the loading curve shown by the interface using Hertz contact law (Eq. (3)).

Fig. 2 Measurement of Young's modulus of an iron ore granule sample.

Time step is another important model parameter in terms of simulation accuracy. Adopting a time step much smaller than its critical value (which is determined by the property of granules) can effectively reduce the effect of residual kinetic energy on the stability of a system to an extremely low level. Furthermore, the adoption of a relative small time step also helps increase the numerical stability of the modelling work, in particular for a dynamic process. The critical time step was evaluated from the equation proposed by Thornton and Randall [60] and was based on the propagation of Rayleigh waves [61]:

$$\Delta t_c = \frac{\pi \cdot R_{\min}}{0.163\sigma + 0.8766} \sqrt{\frac{\rho}{G}} \quad (11)$$

where $R_{\min}$ is the minimum particle radius in the simulation, ρ is particle density.

3. Studies of iron ore granule packing

3.1 Simulation work

Figure 3 shows the initial configuration of the granules (Fig. 3(a)) and the formation of a pile after the discharging process has finished (Fig. 3(b)). The simulations started with the random generation of 10000 iron ore granules, which were simulated as single particles, with sizes ranging from 2.0 mm to 10.0 mm. The corresponding granule size distribution is shown in Table 1. Within each size range, the radius of each particle was randomly generated. Under the influence of gravity, these generated granules fell onto the middle plate, contacted each other and settled to form a granule bed (Fig. 3(a)). Then, the instantaneous opening of a central outlet of the middle plate initiated the discharging process. During this period, a portion of granules flowed downwards and dropped onto the bottom of container to form a pile. The simulation continued until no more granules dropped from the middle plate and the number of contacts and the residual kinetic energy of the granules became stable (Fig. 3(b)). Finally, an in-house developed graphic software was used to visualise the simulation and perform the data analysis. The dimensions of the rectangular container used in the simulation are shown in Table 2.

Table 1. Size distribution of the multi-sized granules generated in the simulation.

Size range	2.0~4.0 mm	4.0~6.0 mm	6.0~8.0 mm	8.0~10.0 mm
Weight percentage (%)	18.2	35.8	27.2	18.8
Number of particles	5000	3400	1150	450

Fig. 3 Simulation of granule packing in a rectangular container. (a) initial condition; (b) pile formation.

Table 2. Dimensions of the rectangular container designed in the simulation.

Dimensions of the container	Value
Container width (m)	0.20
Container thickness (m)	0.05
Container height (m)	0.45
Height of middle plate (m)	0.20
Width of central outlet (m)	0.04

3.2 Experimental work

In order to validate the developed model, the corresponding experiments of iron ore granule packing were carried out under similar conditions to those used in the simulation. The dimensions of the rectangular container used in the experiment, including width, thickness and height, were proportional to those designed in the simulation. The ratio of the experimental to the simulated test rig was 2:1. Furthermore, the total mass of iron ore granules used in the simulations corresponded to the scaled down mass of granules used in the experiments.

Fig. 4 Corresponding experiment of iron ore granule packing. (a) initial condition; (b) pile formation.

In the experiments, a group of iron ore granules were cascaded onto the middle plate of the container to form a bed of granules (Fig. 4(a)). The subsequent discharging process was similar to that of the simulation. When the discharge process finished (Fig. 4(b)), the angle of repose and the level of granule size segregation were measured in sequence. The angle of repose was calculated based on the photos taken in the test using the image-processing software KS400 (developed by Kontron Electronic GMB). This software converted the photos into indexed images. By analysing the images, the inclination of the pile slope was obtained by fitting the coordinates of the centres of the most external granules to either linear or nonlinear functions. Then, the first derivatives at the particle centres were calculated and the slope of the pile was estimated by averaging the values of these slopes. To measure the level of granule size segregation, the formed pile was divided into five sections having the same mass in the horizontal and vertical directions. On removing each section and after screening, the weight percentage of the iron ore granules in each size range was determined. Thus, the granule size segregation was quantified based on the average mass-based granule size in each section. To minimize the measurement error, the pile formation experiments were carried out in quintuplicate. Then, the averaged experimental indices were compared with the ones predicted by the simulation.

4. Results and discussion

4.1 Identification of granule parameters

Figure 5 shows the measurement results of particle size distribution and the apparent density of the sample iron ore granules. The data indicate that the size of iron ore granules was mainly concentrated in the range from 2.0 mm to 10.0 mm. The fraction under 2.0 mm and over 10.0 mm was less than 10 wt.%. The apparent density of iron ore granules fluctuated slightly within the range from 2.8 g/cm³ to 3.2 g/cm³, varying with the specific material properties of individual granule samples. Based on the measurement data, the diameters of the modelled granules were chosen within the range of 2.0-10.0 mm and the corresponding size distribution was set in accordance with the one measured in the experiment. The apparent density was set at a constant value of 3.0 g/cm³ due to its relative steady variation as a function of granule diameter and for modelling simplification.

Fig. 5 Analysis of iron ore granule samples: (a) Cumulative size distribution; (b) Apparent density. The samples used to measure the apparent density were randomly chosen within the size range of 2.0-10.0 mm.

Figure 6 shows the measurement results of the Young's modulus of the sample iron ore granules. As indicated by Fig. 6(a), in most cases of the Young's modulus tests, a compression process includes three stages. First, the piston compresses the adhering layer (Stage A) which is at the outer part of the granule and is usually weaker than the granule core. After the adhering layer breaks, the piston keeps compressing the core of the granule (Stage B) until it is crushed at a certain level (Stage C). In this study, the Young's modulus of the sample granule was calculated based on the data at Stage A because, in terms of contact force calculation, the contact area between the piston and the granule is located at the surface of the adhering layer. Furthermore, in terms of time step determination, the surface waves account for the largest part (67%) of the radiated energy [61], so the Young's modulus of the adhering layer of a granule is also a necessary parameter for calculating the critical time step based on the theory of surface waves propagation. By adopting the relationship between the compression force and granule indentation shown at Stage A, the elastic modulus of the sample granule could be estimated based on the Hertz contact law shown in Eq. (3). Fig. 6(b) shows the measured Young's modulus of ten sample granules within the size range of 2.0-10.0 mm. The average value, $E_{avg} = 33.0$ MPa, was adopted in the simulation study.

Fig.6 (a) Test data obtained from one Young's modulus measurement test; (b) Measured Young's modulus of ten iron ore granule samples.

The other material parameters of iron ore granules were deliberately referred from the literature on the study of iron ore granules or iron ore pellets [25, 62-66]. All the detailed information on the material parameters of iron ore granules adopted in the simulation is summarised in Table 3.

Table 3. Material parameters of the iron ore granules in the model.

Property parameter	Symbol	Value
Granule diameter (mm)	d	2.0-10.0
Granule density (g/cm ³)	ρ	3.0
Young's modulus (MPa)	E	33.0
Poisson's ratio [62, 64, 65]	σ	0.3
Coefficient of restitution [25]	e	0.15
Sliding friction coefficient [62, 64, 65]	μ_s	0.5-0.7*
Rolling friction coefficient [25, 63, 66]	μ_r	0.2-0.3*
Time step (s)	Δt	1.0×10^{-6}

4.2 Influence of friction coefficients on the angle of repose

As shown in Table 3, the sliding and rolling friction coefficients referred from the literature varies within a range because these values are dependent on the type of iron ore granules or iron ore pellets used in measurement test. It is commonly known that sliding friction mainly accounts for the translational kinetic energy dissipation of granules during pile formation and rolling friction represents the dissipation of the angular kinetic energy of rolling granules. Therefore, it is important to investigate the influence of these friction coefficients on the packing stability of iron ore granules. To identify the influence, we carried out a series of simulation trials by setting a value range and a base value for each friction coefficient. (See Table 4).

Table 4 Friction coefficients studied and their value ranges.

Parameters	Base value	Value range
Sliding friction coefficient, μ_s	0.5	0.3-0.7
Rolling friction coefficient, μ_r	0.3	0.1-0.5

4.2.1 Sliding friction coefficient

Five values of sliding friction coefficient ranging from 0.3 to 0.7 were adopted in the simulation cases of granule packing to study its effect on the angle of repose. The visualisations of the simulated results are shown in Fig. 7 and the variation of the simulated angle of repose as a function of sliding friction coefficient is shown in Fig. 8. As the sliding friction coefficient cannot be manually varied in the experiments (as it is a material property), no comparison with corresponding experiments was provided.

Fig. 7 Granule piles formed in five cases with increasing sliding friction coefficient: (a) $\mu_s = 0.3$; (b) $\mu_s = 0.4$; (c) $\mu_s = 0.5$; (d) $\mu_s = 0.6$; (e) $\mu_s = 0.7$.

The data in Fig. 8 show that there is a clear upward trend in the angle of repose with the increase of sliding friction coefficient. The angle of repose went up by about 7.5 degrees when the sliding friction coefficient increased from 0.3 to 0.7.

Fig. 8 Relationship between the simulated angles of repose and sliding friction coefficient.

4.2.2 Rolling friction coefficient

Fig. 9 Granule piles formed in five simulation cases with increasing rolling friction coefficient: (a) $\mu_r=0.1$; (b) $\mu_r=0.2$; (c) $\mu_r=0.3$; (d) $\mu_r=0.4$; (e) $\mu_r=0.5$.

Furthermore, another group of five simulation cases with increasing rolling friction coefficient were carried out and the simulated piles are shown in Fig. 9. The data in Fig. 10 show the relationship between the simulated angles of repose and rolling friction coefficient. It can be seen that the angle of repose went up by about 9.0 degrees when the rolling friction coefficient increased from 0.1 to 0.5.

Fig. 10 Relationship between the simulated angle of repose and rolling friction coefficient.

The upward trends shown in Fig. 8 and Fig. 10 indicate that both the sliding and rolling friction coefficients have a significant influence on the angle of repose of iron ore granules. It is expected that an increase in either the sliding or rolling friction coefficient would, to a large extent, enhance the stability of the granule packing. This can be explained by the following reasoning: firstly, a larger sliding friction coefficient can effectively dissipate the kinetic energy of the discharged granules through interparticle contacts and thus a pile of higher potential would be formed [32]; secondly, increasing the sliding friction coefficient results in a higher angle of internal friction for the granules, which, according to the Mohr–Coulomb failure criterion [67], would increase the shear strength of the granules inside the pile and thus enhance their support for the granule load in the shear direction; thirdly, in terms of energy dissipation, rolling friction has a similar function to that of sliding friction. A larger rolling friction coefficient represents larger rolling resistance opposing to the rotational motion of the granules, thus resulting in more dissipation of the rotational energy in a shorter time.

Furthermore, the increasing rate shown in Fig. 10 is more significant than that shown in Fig. 8. It is likely that during the packing process, the rolling friction coefficient plays a more important role than sliding friction coefficient in preserving the stability of the granule packing.

4.3 Friction coefficients optimization

The results in Section 4.2 demonstrate a significant influence of the friction coefficients on the angle of repose. Therefore, to guarantee the simulation accuracy, the friction coefficients of the iron ore granule samples used in this study should be determined. Given the granule parameters adopted in the references [25, 62-64], we originally set the ranges of sliding and rolling friction coefficients 0.5 ~ 0.7 and 0.2 ~ 0.3 respectively and then selected the optimal combination of friction coefficients of iron ore granules through a series of tuning tests. This is especially necessary when some important model parameters are uncertain or difficult to measure through experiments.

We first carried out the simulations of multi-sized granule packing using six different friction coefficient combinations named from C1 to C6. Simultaneously, the experimental tests of granule packing were carried out as well. The left and right angles of repose measured in each repetitive test are shown in Table 5. Figure 11 shows the comparison between the average experimental angle of repose and the simulated ones obtained using different friction coefficient combinations. The data indicate that the simulated angles of repose of C2, C4 and C5 match the experimental one relatively well because all their simulation errors are within 1.0 degree. However, compared to C2 and C4, C5 matches the experimental data better with the simulation error of only about 0.3 degree. Therefore, C5 ($\mu_s = 0.5, \mu_r = 0.3$) was temporarily considered as the optimal friction coefficient combination.

Table 5 Left and right angles of repose obtained from five repetitive experimental tests.

	Test 1	Test 2	Test 3	Test 4	Test 5
Left angle (°)	36.2	36.1	35.5	35.7	36.0
Right angle (°)	36.0	35.8	35.7	36.1	35.8

Fig. 11 Comparison between the average experimental angle of repose and the simulated ones obtained using different friction coefficient combinations. The experimental data in the chart is the average of the angles of repose shown in Table 5.

Furthermore, we also compared the simulated angle of repose of mono-sized iron ore granules with the experimental result when the granule size increased from 5.0 to 9.0 mm. Fig. 12 shows the experimental trend and the simulated ones obtained using the friction coefficient combinations C1~C6.

It can be seen that the simulated angles of repose for C2, C4 and C5 are still a better match to the experimental result than other combinations. While in comparison to C2 and C4, the data of C5 are closer to the experimental ones especially when $d \geq 7.0$ mm. The simulation errors of C2, C4 and C5 were quantified using a parameter s which is expressed as:

$$s = \sqrt{\frac{1}{5} \sum_{d=5}^9 (x_{\text{sim},d} - x_{\text{exp},d})^2} \quad (12)$$

where $x_{\text{sim},d}$ and $x_{\text{exp},d}$ refer to the simulated and experimental average angles of repose for granule size d . By substituting the data shown in Fig. 12 into Eq. (12), we obtained the simulation errors of C2, C4 and C5 and their values are 0.73, 0.55 and 0.32 respectively. This result shows that the simulated angle of repose obtained using C5 is indeed closer to the experimental data than that using any other friction coefficient combination.

Fig. 12 Comparison of the experimental trend in the average of left and right angles of repose with the increase of granule size and the simulated trends obtained using different friction coefficient combinations.

In summary, both comparisons shown in Fig. 11 and Fig. 12 demonstrate that C5 ($\mu_s = 0.5$, $\mu_r = 0.3$) is the optimal friction coefficient combination for the tested iron ore granules. Therefore, the sliding and rolling friction coefficients were determined as 0.5 and 0.3 respectively in the following simulation tests. The granule piles formed in the experiment and in the simulation test using C5 are shown in Fig. 13.

Fig. 13 Granule piles formed in the simulation test using C5 (left) and in the experiment (right) respectively. The experimental image was chosen from one of five repeated measurement tests.

4.4 Influence of granule size on the angle of repose

In Section 4.3, Figure 12 shows that the angle of repose decreases with granule size. In this section, the comparison between the experimental and simulated angles of repose using C5 (as extracted from Fig. 12) is presented in Fig. 14 in more detail. Fig. 14 shows that the simulated angle of repose decreased by about 4.0 degrees as the granule size increased from 5.0 mm to 9.0 mm. The experimental results also show a similar downward trend throughout the selected size range. The experimental data were obtained from three corresponding experimental tests of granule packing with the size range of 4.0-6.0 mm, 6.0-8.0 mm and 8.0-10.0 mm respectively. The iron ore granule piles formed in the simulation and experimental tests are shown in Fig. 15 and Fig. 16, respectively.

Fig. 14 Relationship between the angle of repose and granule size. The left and right angles of repose obtained from the simulation and experimental tests were compared.

This relationship can be probably explained by the assumption that as granule size increases (from 5.0 to 9.0 mm), the kinetic energy dissipation rate of the discharged granules slowed down during the packing process. Zhou *et al.* [32] originally studied the variation in the total energy dissipation due to friction during a packing process. They (Zhou *et al.* [32]) observed that an increase in particle size was associated to a decrease in the dimensionless sliding friction force and rolling friction torque acting on a given granule.

Fig. 15 Granule piles formed in five simulation cases with increasing granule size d : (a) $d=5.0$ mm; (b) $d=6.0$ mm; (c) $d=7.0$ mm; (d) $d=8.0$ mm; (e) $d=9.0$ mm.

Fig. 16 Granule piles formed in three experimental tests with increasing average granule size: (a) size ranging from 4.0 to 6.0 mm; (b) size ranging from 6.0 to 8.0 mm; (c) size ranging from 8.0 to 10.0 mm.

Fig. 17(a) Variations in the kinetic energy of granules during packing process for five different sizes. The granules start to flow downward from the middle plate at 0.8 s and form a steady pile at the bottom box at 3.0 s. Note: The different peak values of E_k in these five cases are due to that the mass of the discharged granules is slightly different for five different sizes.

Fig. 17(b) Variations in the average number of interparticle contacts, defined as $\bar{n} = \sum_{i=1}^N n_i / N$ (N is the real-time number of discharged granules and n_i is the number of interparticle contacts of granule i), during packing process for five different sizes.

In order to further investigate the observations by Zhou *et al.* [32], we have plotted the kinetic energy (Fig. 17(a)) and the average number of interparticle contacts (Fig. 17(b)) as a function of time for five different granule sizes. The data in Fig. 17(a) indicate that the kinetic energy of a finer granule drops at a faster rate than that of a larger granule. For example, at the end of the discharging process ($t = 1.8$ s), the kinetic energy of the finest granules ($d=5.0$ mm) has dropped to about 0.1 J while that of the largest granules ($d=9.0$ mm) was still about 0.35 J. The results shown in Fig. 17(b) illustrate that the average number of interparticle contacts of the finer particles is larger than that of a coarser one during the whole packing process (from 0.8 to 3.0 s). The comparison of Figs. 17 (a) and (b) suggests that the kinetic energy dissipation rate of the discharged granules is very likely related to the average number of interparticle contacts during the packing process. Therefore, an increase in granule size indeed has an influence on the kinetic energy dissipation rate of iron ore granules and thus affects the packing stability.

4.5 Size segregation of iron ore granules

Size segregation is the result of the different behaviour of granules of different sizes during a particle packing process. As described in Section 3.2, in both simulations and experiments, a mixture of iron ore granules with sizes from 2.0 to 10.0 mm were originally cascaded onto the middle plate of the container, then discharged from the outlet and finally formed a granule pile at the bottom of the container. To quantify the size segregation within the pile, the average mass-based granule size d_m in each divided section of the piles formed in the experiment and simulation was calculated respectively. The schematic diagram shown in Fig. 18 illustrates how the pile was divided into sections. The granule pile was first outlined based on its profile and then, the enclosed area was divided into five even sections. All sections possessed the same area to guarantee equal granule mass sampling.

The simulated d_m of each section was calculated based on the size and final position of each granule recorded in the output file. From these data, the weight percentage of granules in each size range could be obtained. The experimental d_m was calculated by sieving the granules in each section

of the pile and then weighing the granules in each size range in each section respectively. In this study, the expression of the average mass-based granule size in the i th divided section $d_{m,i}$ is given by:

$$d_{m,i} = \sum_{j=1}^4 (W_{i,j} \cdot D_{m,j}) \quad (13)$$

where $D_{m,j}$ is the average size of the granules in the j th size range (For the experimental $D_{m,j}$, it is respectively assumed as 3.0, 5.0, 7.0 and 9.0 mm in the four size ranges). $W_{i,j}$ is the weight percentage of the granules in the j th size range in the i th section:

$$W_{i,j} = m_{i,j} / m_i \times 100\% \quad (14)$$

where $m_{i,j}$ is the mass of the granules in the j th size range in the i th section and m_i is the total mass of the granules in the i th section.

Fig. 18 The schematic diagram showing the divided sections used to calculate the size segregation: (a) in the horizontal direction; (b) in the vertical direction.

4.5.1 Horizontal size segregation

Table 6 Simulated (left) and average experimental (right) weight percentages of the granules in each size range in each section.

Size range	Section 1 (%)	Section 2 (%)	Section 3 (%)	Section 4 (%)	Section 5 (%)	W^* (%)
8-10 mm	22.4, 20.8	18.8, 18.3	15.3, 16.1	16.7, 18.6	22.0, 20.0	18.8
6-8 mm	28.2, 27.6	27.8, 27.3	26.1, 26.2	26.8, 26.6	27.0, 28.2	27.2
4-6 mm	33.8, 34.8	35.0, 35.5	37.1, 36.3	36.4, 36.4	34.5, 35.2	35.8
2-4 mm	15.6, 16.8	18.4, 18.9	21.5, 21.4	20.1, 18.4	16.5, 16.6	18.2

Note: W^* refers to the initial weight percentage of the iron ore granules in each size range (as shown in Table 1).

Fig. 19 Simulated (left) and average experimental (right) weight ratios in each divided section of granule pile.

Table 6 shows the weight percentage of the granules in each size range in each section obtained from the simulated and experimental results, respectively. The corresponding column chart is shown in Fig. 19. By substituting W_{ij} (shown in Table 6) into Eq. (13), the simulated and experimental $d_{m,i}$ were obtained as shown in Fig. 20.

Fig. 20 Comparison of the simulated (left) and experimental (right) average mass-based granule size in each divided section.

The simulated and experimental data in Fig. 20 show similar trends in the values of $d_{m,i}$ in these five divided sections. From the outer sections (Section 1 and 5) to the central section (Section 3), $d_{m,i}$ gradually decreases to the minimum value of about 5.70 mm. This trend indicates that the average granule size is relatively larger in the outer sections than that in the inner sections of the pile. There are mainly two reasons for such horizontal segregation: firstly, as granules flow together along the surface, the smaller granules are more likely to get stuck in the roughness of the surface composed of larger granules and this results in a central core of smaller granules in the pile; secondly, during discharging process, the larger granules preferentially run for a longer distance downward the slope of pile and settle at the bottom due to their higher momentum compared to that of the finer ones.

A parameter λ [64], which is expressed as the difference of dimensionless $d_{m,i}$, is introduced to quantify the horizontal size segregation:

$$\lambda = (d_{m,\max} - d_{m,\min}) / d_m^* \quad (15)$$

where $d_{m,\max}$ and $d_{m,\min}$ are the maximum and minimum $d_{m,i}$ of these five divided sections. d_m^* is the average mass-based size of total iron ore granule mixture and, based on the size distribution shown in Table 1, its value is estimated as 5.80 mm. By applying $d_{m,\max}$, $d_{m,\min}$ and d_m^* to Eq. (15), the simulated and experimental levels of horizontal size segregation were calculated as 0.07 and 0.06 respectively. It can be seen that the simulated λ is very close to the experimental one.

4.5.2 Vertical size segregation

Similarly, the vertical size segregation was quantified by calculating the simulated and experimental d_m of each divided section (shown in Fig. 18(b)) of the pile. The weight percentage of the granules in each size range in each section obtained from the simulated and experimental results is shown in Table 7. The corresponding column chart is shown in Fig. 21. Finally, by substituting W_{ij} into Eq. (13), the simulated and experimental $d_{m,i}$ were obtained as shown in Fig. 22.

Table 7 Simulated (left) and average experimental (right) weight percentages of the granules in each size range in each section.

Size range	Section 1 (%)	Section 2 (%)	Section 3 (%)	Section 4 (%)	Section 5 (%)	W^* (%)
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8-10 mm	20.0, 19.6	19.4, 18.6	18.6, 18.0	18.1, 18.7	16.5, 16.2	18.8
6-8 mm	26.5, 26.2	26.5, 26.8	27.4, 26.8	28.2, 27.6	28.0, 28.7	27.2
4-6 mm	34.0, 33.6	34.1, 34.4	37.2, 38.0	37.2, 36.5	37.5, 37.9	35.8
2-4 mm	19.5, 20.6	20.0, 20.2	16.8, 17.2	16.5, 17.2	18.0, 17.2	18.2

Note: W^* refers to the initial weight percentage of the iron ore granules in each size range (as shown in Table 1).

Fig. 21 Simulated (bottom) and average experimental (top) weight ratios in each divided section of granule pile.

From the data shown in Fig. 21, we can gather a few important features. Firstly, from the top layer to the bottom layer, the weight percentage of the larger granules (8-10 mm) gradually increases. This is because the larger granules possess a higher flowability and tend to roll down along the slope, accumulating at the lower sections of the pile. Secondly, from the top layer to the bottom layer, the weight percentage of the smaller granules (2-4 mm) decreases first and then increases to a higher value. The reason for this trend is that compared to Section 3 and 4, the smaller granules, with a lower flowability, have a relatively larger fraction in Section 5. During the piling process, a part of the smaller granules in the upper layers (Section 3, 4 and 5) percolate through the voids formed by the larger granules, descend and settle at the bottom layers (Section 1 and 2) of the pile. Thirdly, the weight fractions of the smaller intermediate granules (4-6 mm) in the upper layers are larger than those in the bottom layers. This is probably because the granules of this size range still have relatively lower flowability compared to the larger granules and most of them cannot percolate through the voids and descend to the bottom layers due to their relatively larger sizes.

The data in Fig. 22 show that from the top layer (Section 5) to the bottom layer (Section 1), the average mass-based granule size $d_{m,i}$ first increases to its maximum value of about 6.00 mm and then decreases to the minimum value of about 5.85 mm and finally slightly increases to about 5.90 mm. This segregation observed trend is not as significant as the horizontal one.

Fig. 22 Comparison of the simulated (bottom) and experimental (top) average mass-based granule size in each divided section.

Based on the above analysis, it can be seen that the vertical segregation of the granules of each size range may not be clearly reflected by the segregation trend in the average granule size shown in Fig. 22 because this trend is the result of the interaction of multiple segregation mechanisms in the granule packing. For instance, although a large fraction of the larger granules (8-10 mm) accumulate at the base of the pile, the average granule size in Section 1 is still smaller than the values for Section 3 and 4, because there is a larger fraction of the smaller granules (2-4 mm) settling at the bottom layer as well. Nevertheless, the average granule size can still be regarded as a parameter reflecting the general size distribution of the granule mixture in each section of the pile.

Based on the $d_{m,i}$ shown in Fig. 22, the simulated and experimental levels of vertical size segregation were calculated by applying Eq. (15) and the values are 0.03 and 0.02 respectively. The simulated λ is still close to the experimental one but the values are relatively smaller than the ones of horizontal size segregation.

5. Conclusions

A nonlinear DEM model for predicting the behaviour of iron ore granules was developed and validated through a series of comparative numerical-experimental tests of granule pile formation. The influence of granule size, sliding and rolling friction coefficients on the angle of repose of iron ore granules was studied. The size segregation of iron ore granules in the horizontal and vertical directions were investigated both numerically and experimentally.

The influence of the sliding and rolling friction coefficients on the angle of repose was first numerically studied. The simulation results show that as the sliding coefficient increased from 0.4 to 0.8, the angle of repose rose by about 8.0 degrees. When the rolling friction coefficient increased from 0.1 to 0.5, the angle of repose rose by about 9.0 degrees. This was mainly due to the increase in the kinetic energy dissipation rate during the discharging process and the resultant enhanced packing stability of iron ore granules.

To determine the suitable values of the sliding and rolling friction coefficients, we carried out a series of tuning tests in which we compared simulated and experimentally obtained angles of repose. The suitability of any given combination of sliding and rolling friction coefficients was evaluated by using a parameter s . The results showed that the simulated angle of repose obtained using sliding and

rolling friction coefficients of 0.5 and 0.3, respectively minimised the simulation errors as determined by 0.32.

Based on the simulation and the experimental results, the granule size has been demonstrated to have a significant influence on the angle of repose. When granule size was increased from 5.0 mm to 9.0 mm, the angle of repose decreased by about 4.0 degrees. This was attributed to the decrease in the average number of interparticle contacts during the packing process that slowed down the kinetic energy dissipation of the discharged granules and thus decreased the packing stability.

Both the simulation and the experimental results show the size segregation of the iron ore granules in the pile. In the horizontal direction, the average granule size in the outer sections of the pile was relatively larger than that in the inner sections. The reasons are that during the discharging process, the smaller granules tend to get stuck onto the rough surface of the pile and the larger granules preferentially run for a longer distance along the slope of the pile due to their higher momentum. In the vertical direction, the segregation trend was not as significant as in the horizontal one. This was probably due to the interaction of multiple segregation mechanisms during the granule packing, such as the accumulation of larger granules at the bottom of the pile due to their higher momentum and the percolation of smaller granules through voids from the top to bottom of the pile. Finally, the agreement between the simulated and experimental levels of size segregation demonstrated that the developed DEM model was able to be used as a tool to simulate the behaviour of iron ore granules during packing process.

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