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A Monte Carlo simulation method for estimating the fine rattler fraction in large-ratio binary mixtures

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Abstract: Reliable estimation of the fine particle rattler fraction is crucial for understanding the structural and mechanical responses of binary granular systems with large size ratios. However, such estimation is challenged by the general inability to obtain interparticle contact force information directly from experimental images and by the lower accuracy of positional and size identification of fine particles compared with coarse particles. To address these challenges, in this study we focused on two-dimensional (2D) bidisperse granular assemblies with large size ratios (α = 7, 9, 12, and 16) and developed an approach based on Monte Carlo simulation (MCS) that relies solely on the size and positional information of coarse particles, avoiding the need for force-resolved computations. The performance of the method was evaluated against experimental measurements and discrete element method (DEM) simulations. The MCS-based predictions show close agreement with experimental results, with a slight overall overestimation. At low fines content, the approach tends to overestimate the fine particle rattler fraction relative to DEM results, whereas at higher fines content, it underestimates rattler fraction. Overall, the proposed MCS-based approach enables robust and relatively accurate estimation of the fine particle rattler fraction. This study provides a practical framework for predicting rattler fraction, contributes to advancing both experimental analysis and theoretical modeling in granular physics, and demonstrates the conceptual extendibility of the MCS framework to more complex three-dimensional (3D) packings.

Key words: Granular materials; Rattlers; Fines content; Size ratio; DEM; Monte Carlo

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1 Introduction

Binary granular soil mixtures, such as sand–silt and gravel–sand mixtures, are widely used in geotechnical structures including foundations, rockfill dams, and railway ballasts, where their macromechanical properties are essential for structural stability. The macroscopic behavior of these materials is closely linked to their particle-scale interactions. A jammed granular material consists of two coexisting subsets of particles: non-rattlers and rattlers (Behringer and Chakraborty, 2019). A particle is considered a rattler if it has too few contacts to contribute to the mechanical stability of the packing (Santos et al., 2020; Srivastava et al., 2021). Specifically, a particle is typically identified as a rattler if its number of contacts, z_i falls below a critical threshold c ($z_i < c$), where c depends mainly on the system's dimensionality and the presence of interparticle friction. Table 1 summarizes representative values of c reported in previous studies under various dimensional and frictional conditions. For two-dimensional (2D) systems, there is a broad consensus that c = 3 for frictionless particles and c = 2 for frictional ones. In contrast, for three-dimensional (3D) systems, different studies have adopted various values of c even under the same frictional condition.

The number of rattlers directly reflects the mechanical redundancy of a granular system (Huang et al., 2014), and their undifferentiated inclusion can obscure meaningful statistical analyses. Many studies exclude rattlers when computing the structural or mechanical metrics. Thornton (2000),

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Biazzo et al. (2009), Lin et al. (2023), and Ling et al. (2024) excluded rattlers when calculating the average coordination number. Similarly, Zhang et al. (2010) and Berzi and Vescovi (2021) considered only non-rattler particles when evaluating fabric tensors. Huang et al. (2014) and Duverger et al. (2021) treated rattlers as
voids when determining the critical state void ratio, thereby recovering the classical form of the critical state line, in which the void ratio decreases with increasing confining pressure. Moreover, Tejada et al. (2024) corrected the computation of the mean macroscopic stress by scaling the stress tensor σ_{ij} by $1/(1-\eta_r)$, where η_r denotes the rattler fraction, defined as the ratio of rattlers to the total number of particles.

Table 1 Critical coordination number *c* for rattler identification under different dimensionalities and friction conditions reported in previous studies. Note: "n" and "y" indicate frictionless and frictional systems, respectively.

Reference	Dimensionality	Friction	*c*
Babu et al. (2023)	2D	n	3
Petit and Sperl (2025)	2D	n	3
Newhall (2025)	2D	n	3
Majmudar et al. (2007)	2D	y	2
Jiang et al. (2024)	2D	y	2
Lee et al. (2025)	2D	y	2
Lee and Hurley (2025)	2D	y	2
Kumar et al. (2016)	3D	n	4
Yoshii and Otsuki (2025)	3D	n	4
Santos et al. (2020); Srivastava et al. (2021)	3D	n	3
Thornton (2000)	3D	y	2
Thakur et al. (2021)	3D	y	2
Santos et al. (2020); Srivastava et al. (2021)	3D	y	2
Xu et al. (2021)	3D	y	2
Redaelli and Prisco (2019)	3D	y	2
Wautier et al. (2019)	3D	y	1

Although often excluded to reduce statistical distortion, recent studies have highlighted the potentially constructive roles of rattlers in granular mechanics. For example, Wautier et al. (2019), conducted a series of drained triaxial loading simulations using the discrete element method (DEM) with various rattler contents and found that rattlers help stabilize the granular skeleton. Similarly, Hu et al. (2024) showed that rattlers provide lateral support to force chains, thereby enhancing shear strength under confining pressure.

These contrasting roles underscore the importance of accurately estimating η_r. Previous research has shown that η_r is affected by several factors, including particle size distribution (Prasad et al., 2017; Maher and Torquat et al., 2024), confining pressure (Huang et al., 2014; Duverger et al., 2021; Hu et al., 2024), and interparticle friction (Huang et al., 2014; Srivastava et al., 2021). For example, Prasad et al. (2017) simulated random, close-packed binary mixtures of spheres and found that the fine rattler fraction η_r^f (rattlers among fine particles) increases with the size ratio α (coarse-to-fine radius ratio) at a fixed fines content f_c (volume fraction of fine particles), and decreases with f_c at fixed α. Notably, when $\alpha \geq 5.75$ and $f_c < 20\%$, most fine particles are unjammed, causing their η_r^f to approach 100%. In contrast, coarse particles generally remain jammed across all f_c levels because of their relatively large size. Consequently, fine rattlers become the dominant contributor to the total rattler number in systems with large α and low f_c, making their estimation critical for understanding structural and mechanical responses. For 2D isotropic packings with particle size ratios up to ~2, Jiang et al. (2024) showed η_r can be linearly approximated using the mean cell order, regardless of the particle shape.

While the DEM can determine all interparticle contact forces through force-resolved computations and thereby achieve high predictive accuracy in η_r, such mechanical information is generally not directly obtainable from experimental techniques such as X-ray computed tomography (Xia et al., 2017; Cheng and Wang, 2018) or simple optical imaging (Wang et al., 2026). Under a fixed imaging resolution, coarser particles are generally identified with higher accuracy than finer ones (Li et al., 2025). Because experimental images lack direct contact force information, determining whether two particles are actually in contact based solely on size and positional information is inherently challenging (Xia et al., 2017), and the relatively low identification accuracy of fine particles further increases the difficulty of resolving contacts involving them. Although some studies have attempted to infer contact forces indirectly using multi-objective optimization algorithms (Hurley et al., 2016a; Hurley et al.,

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2016b), this was beyond the scope of the present study.

Owing to the inherently stochastic nature of pore networks and particle arrangements, estimating η_r represents a typical uncertainty quantification problem. The Monte Carlo simulation (MCS) method, widely used for uncertainty analysis (Elishakoff, 2003), has been extensively applied in geotechnics (Wang et al., 2010; Wang, 2011; Zhang et al., 2022; Gao et al., 2023). This enables the quantitative assessment of system responses under uncertainty through large-scale stochastic sampling (Hu and Wang, 2020; Li and Wang, 2023).

Although 3D granular assemblies better represent real-world systems, they also involve more complex contact networks. In contrast, 2D packing offers a more tractable framework for investigating particle-scale packing structures and estimating η_r due to its geometric simplifications.

To address the challenges posed by the general inability to obtain interparticle contact force information directly from experimental images of granular packings, as well as the lower positional and size identification accuracy of fine particles compared to coarse particles—both of which hinder the estimation of η_r^f—in this study, we framed the estimation of η_r^f as an uncertainty quantification problem. Focusing on 2D bidisperse granular assemblies with large size ratios (α = 7, 9, 12, and 16), we developed an MCS–based approach that relies exclusively on the size and positional information of coarse particles, without requiring force-resolved computations. The remainder of this paper is organized as follows. Section 2 introduces the MCS method in detail. Section 3 compares the MCS-based predictions with experimental results and DEM data. Section 4 discusses potential extensions and applications of the MCS framework, and Section 5 concludes the study with key findings, limitations, and prospects.

2 Methodology

In this paper, we propose an MCS-based method for estimating the proportion of fine rattlers in binary mixtures. The basic conceptual framework involves first determining the void size distribution within the coarse particle assembly, followed by placing fine particles in these voids and identifying those that meet the floating (rattler) criteria. The overall procedure is illustrated in Fig. 1 and includes the following five steps: (1) extracting the inscribed void size distribution from the coarse particle assembly via Delaunay tessellation, (2) adjusting the inscribed void circle size to match the maximum packing density, (3) classifying the adjusted void circles based on the maximum number of fine particles that they can accommodate, (4) calculating and updating the selection weight of each void category for random fine particle placement, and (5) identifying fine rattlers as those within voids that do not exceed their maximum capacity. This process is repeated 1,000 times to compute the average fine rattler fraction η_r^f. The following subsections elaborate on each step.

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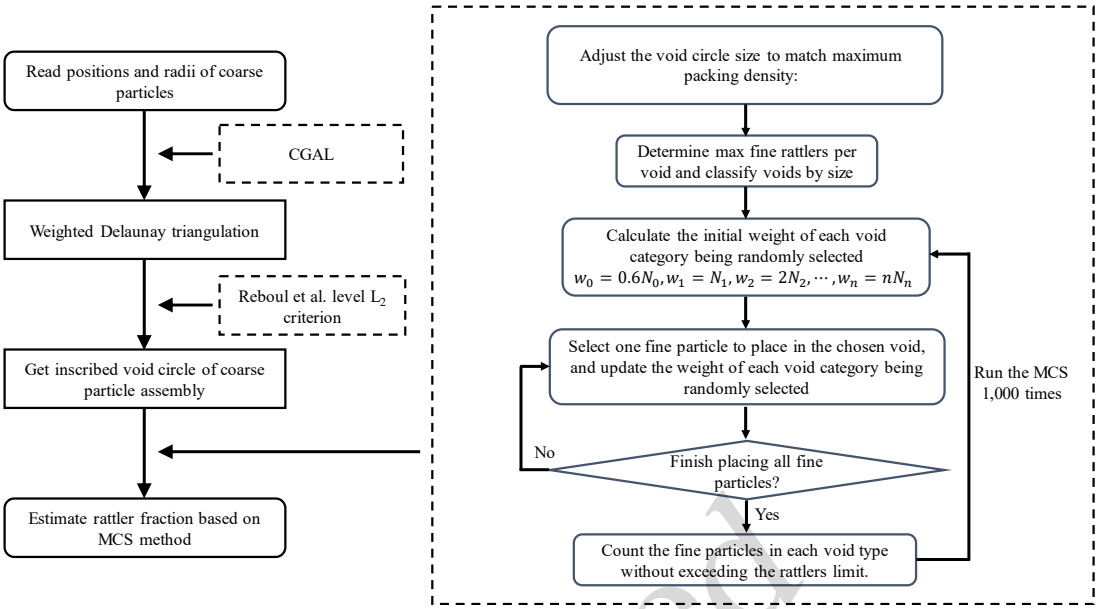

Fig. 1 Calculation procedure for the proposed MCS-based method.

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2.1 Characterization of inscribed void size distribution by Delaunay tessellation

The weighted Delaunay tessellation-based algorithm, originally proposed by Al-Raoush et al. (2003) and Reboul et al. (2008), enables the evaluation of void spaces located within tetrahedra and constrictions on tetrahedral faces, where the constriction size is defined as the diameter of the largest empty disc that can fit between the three particles forming the face, in numerically generated assemblies of 3D polydispersed spheres based on known particle positions and radii (Fig. 2(a)). In our study, we adapted this approach to a 2D granular system, where the packing domain was partitioned using Delaunay triangulation. Each triangle connects the centroids of three neighboring particles (Fig. 2(b)), and triangulation is implemented using the Regular Delaunay algorithm from the CGAL library (https://doc.cgal.org/latest/Manual/packages.html). For each triangle, we then compute an inscribed void circle tangent to the three surrounding particles joined by the triangle under consideration, rather than the inscribed circle of the geometric triangle itself, as illustrated by the blue-line circles in Fig. 3. The radius of this circle provides a useful estimate of local void size (Bryant et al., 1993; Reboul et al., 2008; Nguyen et al., 2021).

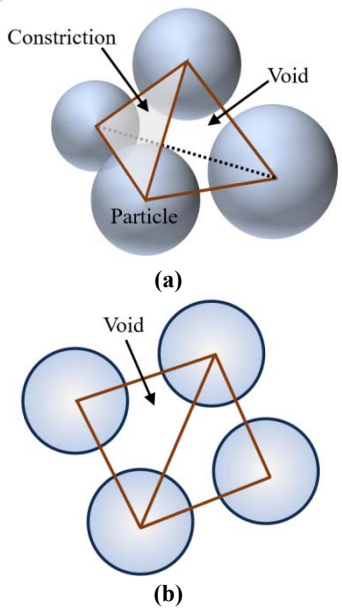

Fig. 2 Illustration of Delaunay cells: (a) a 3D Delaunay cell: the tetrahedron is built from the centers of four neighboring particles. The void corresponds to the volume inside the tetrahedron, while the constrictions are associated with the faces of the cell (one of which is shaded in the figure); (b) a 2D Delaunay cell: the triangulation is built from three neighboring particles.

To prevent the over-segmentation of voids, Reboul et al. (2008) and Reboul et al. (2010) introduced two merging criteria, L_1 and L_2. The L_1 criterion considers a central triangle and its immediate neighbors (triangles labeled L_1 in Fig. 3),

while the L_2 criterion extends this by including the next-nearest neighbors—i.e., the neighbors of the L_1 triangles (triangles labeled L_2 in Fig. 3). Merging decisions are based on the relative overlap γ, defined as $\gamma = \frac{\delta}{\min(d_i, d_j)} \in [0,1]$, where δ is the overlap between the void circles, and d_i and d_j are their respective diameters. If γ exceeds the user-specified threshold γ^{th}, the adjacent triangles are merged into one. The selection of γth is somewhat subjective: for instance, Al-Raoush et al. (2003), Shire et al. (2013) and Shire and O'Sullivan (2016) used a 50% overlap threshold, whereas Sufian et al. (2015) adopted a stricter criterion by setting $\gamma^{\text{th}} = 0$, effectively disallowing any overlap. More recently, Nguyen et al. (2021) proposed a merging method with minimal dependence on γ^{th}, which yielded results comparable to those obtained using the L_2 criterion with $\gamma^{\text{th}} = 0$. This consistency across methodologies supports the use of the L_2 criterion with zero overlap as a robust and objective approach for void space characterization.

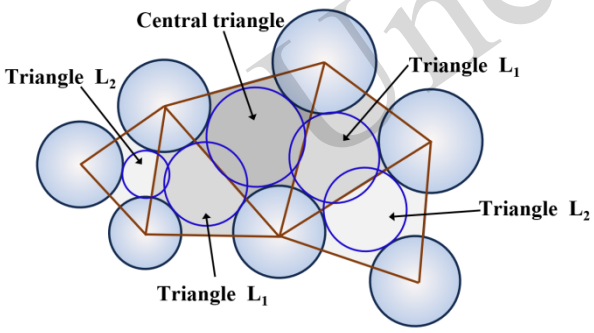

Fig. 3 Schematic diagram of adjacent triangles under the L_1 and L_2 merging criteria, based on Reboul et al. (2008) and Reboul et al. (2010) (adapted from Nguyen et al., 2021). L_2 includes the central triangle, its direct neighbors (L_1), and their neighbors. Note that L_1 is a subset of L_2

Consequently, in this study we adopted the L_2 criterion with $\gamma^{\text{th}} = 0$ to ensure consistent void identification while minimizing the subjective influence during merging. The original code developed by Shire et al. (2013) for computing the constriction size distributions in 3D was modified to suit 2D systems, preserving the core-merging logic. Following Reboul et al. (2008), Roblee et al. (1958), and Reyes and Iglesia. (1991), the analysis domain excludes boundary regions within a lateral distance of two coarse particle diameters to mitigate edge effects. Based on this framework, the distribution of inscribed void circle sizes is determined from the known radii and positions of coarse particles.

2.2 Adjusting the inscribed void size

Because inscribed void circles underestimate the actual void sizes arising from irregular pore shapes, they consequently underestimate the number of fine particles that can occupy the voids (Reboul et al., 2008). As illustrated in the lower right corner of Fig. 4(a), the actual void can accommodate three fine particles, whereas the corresponding inscribed void circle (upper-right) permits only one. In contrast, the void-area-equivalent circle method, which which assumes that voids are completely filled by fine particles (i.e., packing density $\varphi = 1$), tends to overestimate void capacity (Reboul et al., 2008), as illustrated in Fig. 4(b). To strike a balance between these two extremes, the radius of each inscribed void circle is adjusted such that the total void space corresponds to the maximum packing density $\varphi_{\max}$ of a binary mixture with a specific size ratio. This reference value reflects the densest achievable configuration under idealized conditions and provides physically meaningful normalization. This adjustment is formulated as follows:

$$\varphi_g + \pi \sum (s r_v^{\text{ins}})^2 = \varphi_{\max}, \tag{1}$$

where r_v^{ins} is the original inscribed void radius obtained in Section 2.1, s is the size correction factor, and φ_g is the packing density of coarse particles, which is defined as the ratio of the total area of coarse particles to the total area of the system. Thus, the adjusted void radius is given by $r_v^{\text{adj}} = s r_v^{\text{ins}}$ as indicated by the dashed circle in the lower right side of Fig. 4a. The value of $\varphi_{\max}$ is determined using the 3-parameter particle packing model proposed by Kwan et al. (2013), which incorporates both filling and embedment mechanisms. Once the minimum void ratio $e_{\min}$ is known, $\varphi_{\max}$ can be computed as follows:

$$\varphi_{\max} = 1/(1+e_{\min}), \tag{2}$$

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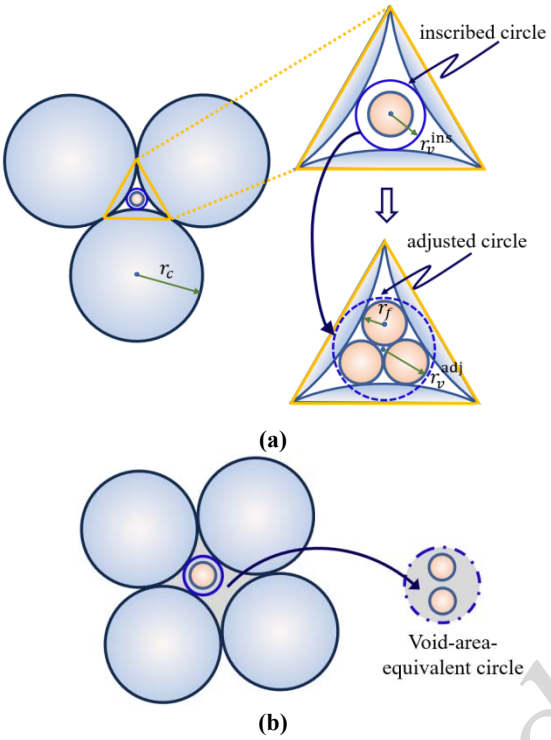

Fig. 4 Schematic illustration of void size adjustment methods: (a) underestimation of the maximum number of fine particles using the inscribed circle method, where r_c is the radius of coarse particles, r_f is the radius of fine particles, r_v^{ins} is the original inscribed void radius and $r_v^{\mathrm{adj}} = sr_v^{\mathrm{ins}}$ is adjusted void radius; (b) overestimation of the maximum number of fine particles using the void area-equivalent circle method. Solid, dashed, and dash-dotted circles represent inscribed circle, adjusted circle, and void-area-equivalent circle, respectively

Figure 5 compares the void ratio e as a function of the fines content f_c for binary mixtures with size ratios α = 7 and 9, obtained from experiments (Wang et al., 2026), and α = 12 and 16, obtained from DEM simulations (detailed in Section 3.2), with corresponding theoretical predictions. The theoretical results show good agreement with both experimental and simulation data across the full range of size ratios considered. At low f_c, the void ratio e decreases as f_c increases. When e reaches its minimum $e_{\min}$, fine particles fully occupy the inter-aggregate voids, representing the transitional or threshold fines content (Lade et al., 1998; Yang et al., 2006). Beyond this point, further increases in f_c lead to an increase in e, indicating the opposite trend. The corresponding threshold fines content f_c^{th}, minimum void ratio $e_{\min}$, and computed $\varphi_{\max}$ values calculated in this study are summarized in Table 2.

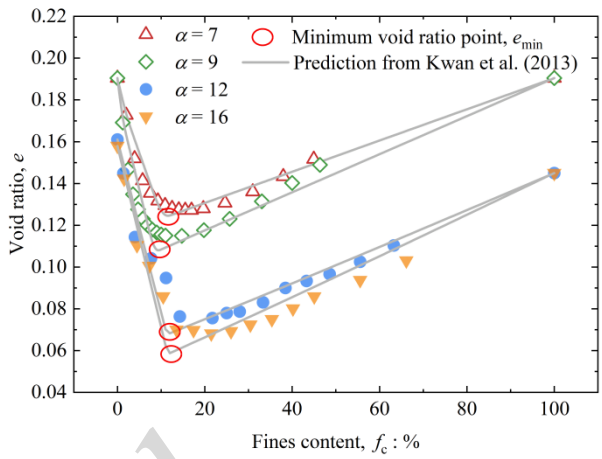

Fig. 5 Comparison of predicted and measured void ratios for binary mixtures with different size ratios α. Experimental data for α = 7 and 9 (Wang et al., 2026) are shown as open symbols, while DEM simulation results for α = 12 and 16 (this study) are shown as filled symbols. Solid curves in both plots show theoretical predictions by Kwan et al. (2013). The red-circled point indicates the minimum void ratio, corresponding to the threshold (or transitional) fines content.

Table 2 The threshold fines content, minimum void ratio, and maximum packing density for different size ratios calculated in this study

Size ratio α (coarse/fine)	Threshold fines content f_c^{th}(%)	Minimum void ratio $e_{\min}$	Maximum packing density $\varphi_{\max}$
7	11.57	0.1249	0.8890
9	9.16	0.1070	0.9033
12	11.31	0.0663	0.9378
16	11.67	0.0568	0.9463

2.3 Classification of adjusted void circles

The *Best Known Packings of Equal Circles in a Circle* database (Otto von Guericke University Magdeburg, 2025) provides optimal configurations for placing equal-sized circles within a larger enclosing circle, along with the maximum number of such circles that can be accommodated for various radius ratios. Here, the radius ratio is defined as the ratio of the adjusted void circle radius r_v^{adj} to the fine particle radius r_f. The number of fine particles that can be accommodated increases in a stepwise manner with r_v^{adj}/r_f within the range [0, 3.81] (Fig. 6(a)). For

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example, a ratio of 2.41 permits a maximum of four fine particles within the void circle. Based on this relationship, the adjusted void circles are classified according to their maximum fine-particle capacities. For each capacity level, the number of corresponding voids is counted—for instance, N_1 and N_4 represent the number of voids that can accommodate one and four fine particles, respectively (Fig. 6(b)). This classification forms the basis for the subsequent calculation of the selection weights for the Monte Carlo placement of the fine particles.

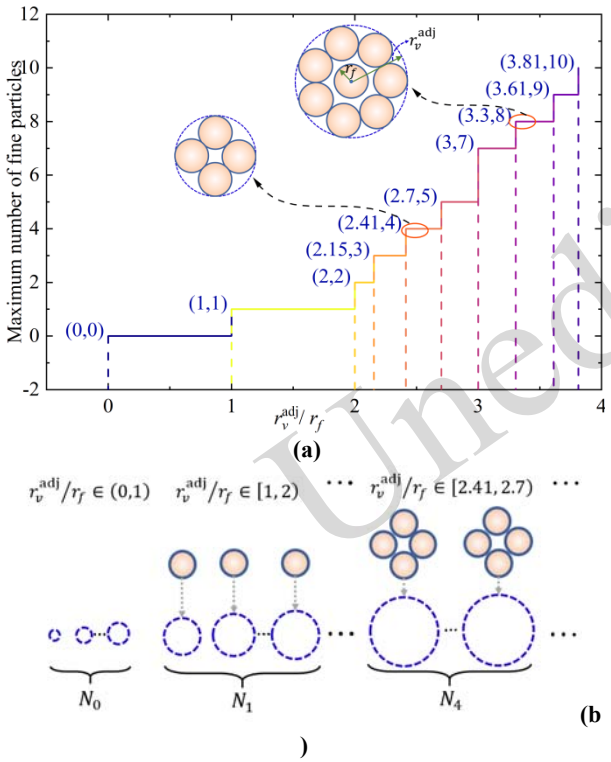

Fig. 6 Schematic diagram of classifying adjusted void circles: (a) the relationship between the maximum number of equal-sized fine particles that can be accommodated and the ratio of the adjusted void circle radius to the fine particle radius (r_v^{adj}/r_f); (b) classification of adjusted void circles according to the maximum number of fine particles they can hold, where Ni denotes the number of void circles that can accommodate i fine particles.

2.4 Initial weight calculation and update of void circles with fine particles

To account for the influence of void size and frequency on the probability of selecting a void for fine particle placement, the initial weight assigned to each void category is defined as $w_i = iN_i$, where i denotes the maximum fine particle capacity of the voids and N_i is the number of voids in the corresponding category (Fig. 7(a)). For small voids where the adjusted radius-to-fine-particle-radius ratio $r_v^{adj}/r_f \in (0,1)$, a scaling factor of 0.6 is applied to reflect their reduced likelihood of being selected. Accordingly, the weight for this group is set as $w_0 = 0.6N_0$. This factor was optimized to match the experimental observations and simulated results (for details, see Supplementary Materials Section 1).

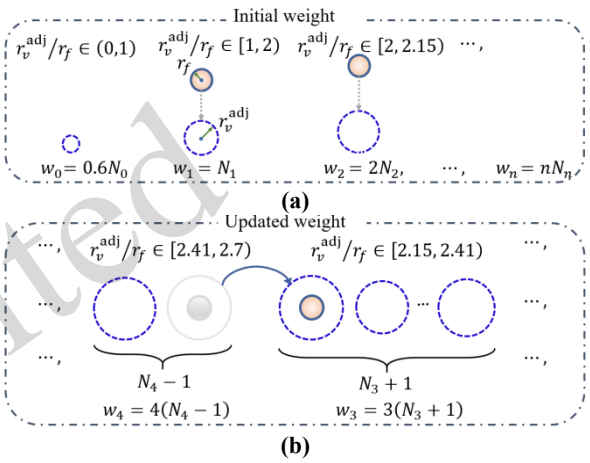

Fig. 7 Schematic illustration of the weight assignment and update process for void circles during fine particle placement: (a) initial weight calculated as the product of the maximum capacity and the number of corresponding void circles; (b) weight update mechanism as fine particles are sequentially placed, with void circles transitioning between categories based on remaining capacity.

The weights are updated dynamically during the Monte Carlo simulation. When a fine particle is placed into a void, the number of voids in that category is reduced by one, whereas the count in the next lower category is increased by one (Fig. 7(b)). The corresponding weights are then recalculated to reflect the updated void circle number distribution. This process is repeated until all fine particles within the valid analysis zone are placed. The total number of fine particles in the assembly is multiplied by the area fraction of the valid region to estimate the number of fine particles within the valid zone. This region excludes a boundary zone extending inward from the edges by a distance of two coarse particle diameters, as defined in Section 2.1. For each void circle, if the number of fine particles placed does not exceed the maximum void capacity, the particles are

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classified as rattlers. The total number of rattlers is recorded for each MCS. As shown in Fig. 8, the predicted η_r^f stabilizes with increasing MCS runs, based on the case of α = 7 and $f_c = 2\%$, which corresponds to one of the lowest fine particle counts among all cases considered in the experiments of Wang et al. (2016) ($N_f = 158$). When this total fine particle number (i.e., number of runs × N_f) exceeds about 1580, the statistical variation in η_r^f falls below 1%, with values confined within a narrow range between 0.71 and 0.72. Based on this convergence behavior, 1,000 was conservatively adopted as the number of MCS runs needed to ensure statistical reliability of the estimated average η_r^f for all binary mixtures.

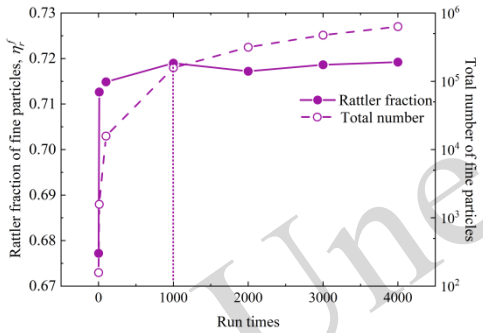
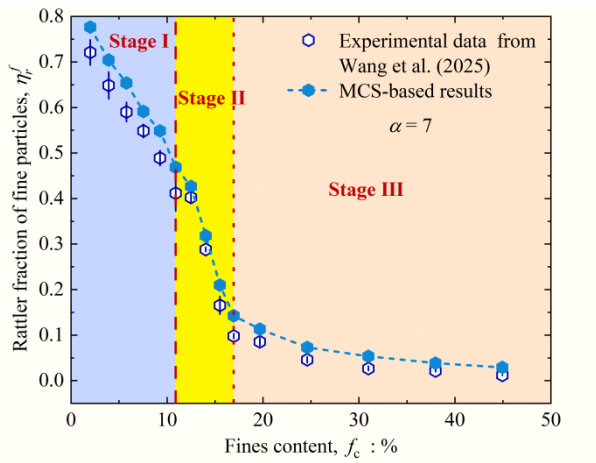


Fig. 8 Convergence behavior of the fine rattler fraction with increasing numbers of MCS runs for the binary mixture with α = 7 and $f_c = 2\%$. Solid symbols indicate the rattler fraction, and open symbols indicate the total number of fine particles in the MCS.

3 Comparison of MCS-based results with experiments and simulations

3.1 Comparison with experimental data

Figure 9 compares the fine rattler fractions η_r^f estimated using the MCS-based method with the experimental results from Wang et al. (2026) for binary mixtures with size ratios of α = 7 and 9 over a range of fines content f_c. Specifically, a series of 2D dense binary packing optical experiments with size ratios α = 3, 5, 7, and 9 were conducted using colored POM disks of fixed thickness. The mixtures were manually prepared in a square Perspex frame placed horizontally on a glass plate to eliminate vertical pressure gradients. Each packing was constructed under high-density conditions, with all four rigid boundaries applying compressive forces to generate a jammed particle network. High-resolution images were processed using Hough transform-based detection and a distance-based contact criterion. Rattlers are defined in the experiments as particles with fewer than three contacts. Overall, the MCS-based estimates showed good agreement with the experimental observations, although they tended to slightly overestimate η_r^f. This deviation arises mainly from the idealized assumption in the MCS method: all fine particles within a void circle are treated as rattlers if their number does not exceed the maximum capacity of the circle. In practice, some of these particles may become mechanically stable due to local geometric constraints, leading to lower actual rattler counts. For instance, Fig. 10 illustrates a case where three fine particles are already mechanically stable in a real void, whereas the corresponding adjusted void circle under the MCS assumption requires at least five particles to achieve a non-rattler configuration.



(a)

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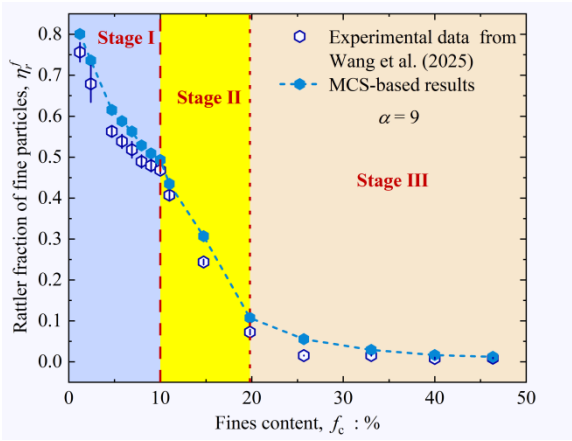


(b)

Fig. 9 Comparison of MCS-based and experimental rattler fractions for the two size ratios (α = 7 and 9): (a) α = 7; (b) α = 9. Open symbols represent measured fine rattler fractions from the experiments, error bars are one standard error of the mean, filled symbols with dashed lines are MCS-based results.

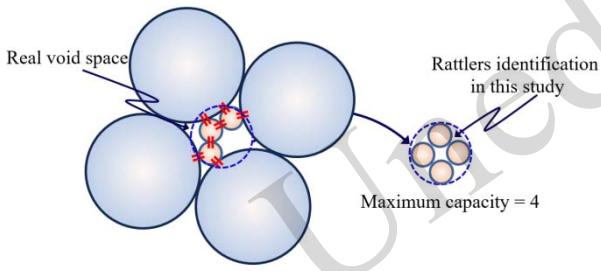
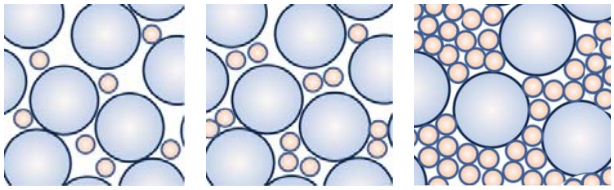


Fig. 10 Diagram of the discrepancy in rattler identification between actual void spaces and the maximum circle capacity assumption used in the MCS method. The dashed circle represents the adjusted void circle, while short red double-solid lines denote contacts between particles and their neighbors.

In addition, the discrepancy is partly attributed to the contact detection criterion used in experimental image processing. Specifically, two particles are identified as being in contact if the distance between their centers satisfies a threshold-based condition. As $\boldsymbol{f_c}$ increases, fine particles become more densely packed (Fig. 11(a) v. 11(c)), making the system more prone to registering apparent contacts between particles that are not actually touching when a fixed threshold is used. This leads to an underestimation of $\boldsymbol{\eta_r^f}$ when applying a coordination-based criterion.



(a) (b) (c)

Fig. 11 Schematic representation of binary granular mixtures with various fines contents: (a) coarse particle-dominated structure, where fines are present in small amounts, insufficient to fill the voids between coarse particles; (b) binary granular mixtures at the lower transitional threshold; (c) fine particle-dominated structure, where coarse grains are scarce, embedded within a matrix dominated by fine particles.

As f_c increases, η_r^f generally decreases. This trend can be divided into three distinct phases (Fig. 9): stage I, a steep decline; stage II, a continued decline with a slight change in slope; and stage III, a gentle reduction. These phases reflect the structural transition of the binary packing system from coarse-to fine-particle dominance (Fig. 11). At low f_c, many fine particles remain unjammed in voids between coarse particles (Fig. 11a), leading to a sharp initial drop in η_r^f (Stage I) as voids begin to fill. When f_c reaches a lower transitional fines content (indicated by the red dashed lines in Fig. 9), many fine particles remain unjammed. A small increase in f_c causes a large fraction of these particles to jam simultaneously (Fig. 11b), leading to another significant decrease in η_r^f (Stage Ⅱ). Eventually, beyond the upper transitional threshold (red dotted lines in Fig. 9), most voids become saturated, and most fine particles attain mechanical stability (Fig. 11c), resulting in a slow decrease in η_r^f (Stage III).

It is important to clarify the definitions used for the transitional fines content. In Fig. 5, the threshold or transitional fines content f_c^{th} is identified as the point at which the trend reverses. In contrast, Fig. 9 defines the lower and upper transitional fines content as the two inflection points in the η_r^f-f_c curve, which delineates the transitional zone. Both the transitional fines contents and the width of the transitional zone vary with size ratio α (Fig. 12). Specifically, the lower threshold tends to decrease with increasing α, whereas the upper threshold generally increases. An exception occurs at $\alpha = 9$, where the upper threshold appears unusually high—likely due to the relatively

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sparse experimental coverage near the upper transitional range, as indicated by the wide spacing between tested fines contents in this region, which limited the accuracy of upper threshold identification. Although the comparative analyses for α = 12 and 16 are discussed in Section 3.2, their data are also included in Fig. 12 for completeness.

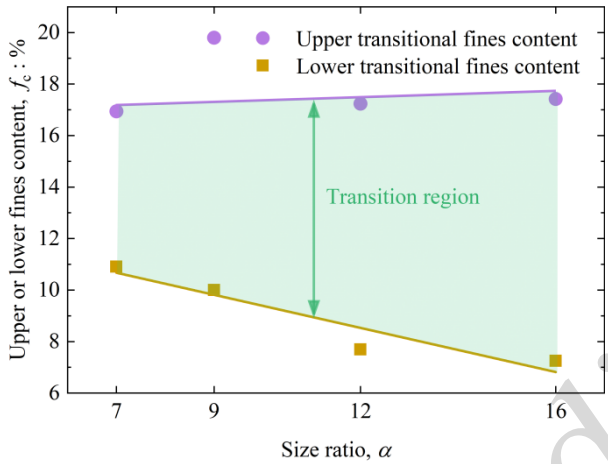

Fig. 12 Lower and upper transitional fines contents as a function of particle size ratio α.

3.2 Comparison with DEM simulations

To further validate the proposed MCS-based method, DEM simulations were carried out on binary mixtures with the four size ratios (α = 7, 9, 12 and 16) subjected to isotropic biaxial compression.

3.2.1 Simulation setup and procedure

DEM simulations were conducted using PFC2D (Itasca Consulting Group, 2014), employing a linear contact model governed by Coulomb friction (Ling et al., 2024; Hu et al., 2024). The model can be expressed as follows:

$$\begin{cases} f_n = k_n \delta_n \\ f_s = \min\{f_{s0} + k_s \Delta\delta_s, \mu f_n\} \end{cases}, \quad (3)$$

where f_n and f_s are the normal and tangential contact forces, respectively; k_n and k_s are the corresponding normal and tangential contact stiffnesses, respectively; f_{s0} is the initial tangential force at the current time step; δ_n represents the normal overlap between particles; and $\Delta\delta_s$ is the incremental tangential displacement. This contact model enables a detailed analysis of both particle-particle and particle-wall interactions (Navarro and de Souza Braun, 2013).

The simulation consists of two stages: sample generation and isotropic loading (Fig. 13). For sample generation, following the criteria of Shire et al. (2014) and Indraratna et al. (2021), each sample contained more than 500 coarse particles to ensure representativeness. The particles were randomly distributed within a square domain bounded by frictionless rigid walls. After the initial configuration was established, an isotropic compression protocol was applied by slowly moving the walls inward under a constant confining pressure of 100 kPa. Compression continued until the system reached mechanical equilibrium, defined by contact force fluctuations below 10^{-5} (Yang and Chu, 2024). Gravity was neglected during the entire process to avoid particle segregation and anisotropy. The representative compositions of the mixtures used in the simulations are presented in Table 3, and a complete list of all simulation cases is provided in Supplementary Materials Table S3. Fine particles with less than three contacts were identified as rattlers, following the convention of previous studies (Babu et al., 2023; Petit and Sperl, 2025; Newhall, 2025).

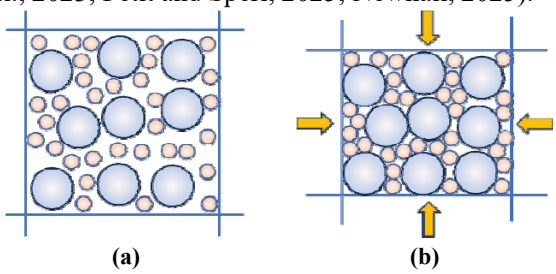

Fig. 13 Schematic diagram of the DEM simulation: (a) sample generation; (b) isotropic compression

Table 3 Representative DEM simulation cases for different size ratios

Size ratio α (coarse/fine)	Fines content f_c (%)	Number of particles
7	2.00	4172
	7.55	10463
	19.67	7883
	24.62	10183
	30.99	17066
	44.94	22837
9	1.22	4382
	7.95	11818
	14.74	7815
	33.06	27921
	46.36	39121
12	1.37	3348
	11.11	19114

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	21.74	32773
	33.33	44614
	38.46	57199
Size ratio α (coarse/fine)	Fines content f_c (%)	Number of particles
	1.54	12536
	10.49	19003
16	21.47	41251
	30.43	66331
	40.19	72474

Note: A complete list of all simulation cases is available in Supplementary Materials Table S3.

3.2.2 Parameter calibration and model validation

To ensure the fidelity of the DEM model, the contact parameters were calibrated by matching the simulated fine-rattler fraction to the experimental observations. The normal contact stiffness k_n can be derived from the effective modulus E^* using the relation $k_n = AE^*/L$, where $A = 2R$, $R = \min\{R^{(1)}, R^{(2)}\}$, and $L = R^{(1)} + R^{(2)}$ (Itasca Consulting Group, 2014; Meshkinghalam et al., 2025). Here, $R^{(1)}$ and $R^{(2)}$ denote the radii of the two particles in contact. The final calibrated parameters are listed in Table 4. Figure 14 presents a comparison of the fine rattler fraction η_r^f obtained from the DEM and experimental measurements for binary mixtures with $\alpha = 7$ and 9, showing good agreement and validating the accuracy of the calibrated model.

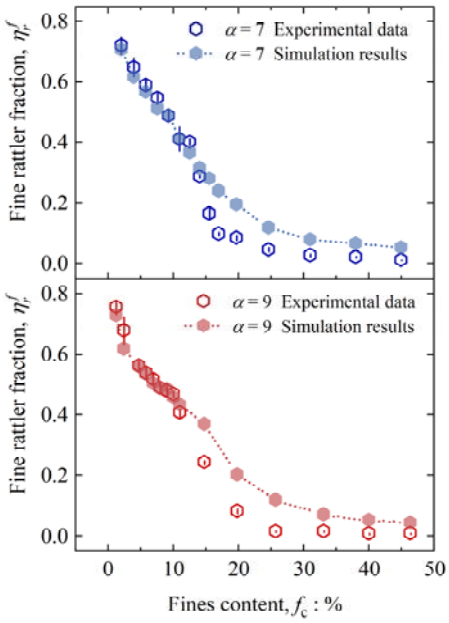

Fig. 14 Comparison of simulated and experimental fine rattler fraction for size ratios $\alpha = 7$ (top) and $\alpha = 9$ (bottom). Open symbols represent measured fine rattler fractions from the experiments, error bars are one standard error of the mean, and solid symbols with dotted lines represent simulation results.

Table 4 Parameters used in the numerical simulation

Parameter	Value
Normal contact stiffness of walls (N/m)	10^9
Effective modulus (Pa)	10^8
Confining pressure (kPa)	100
Stiffness ratio (k_n/k_s)	1.0
Interparticle frictional coefficient	0.0
Wall–particle frictional coefficient	0.0
Particle density (kg/m^3)	2650
Damping coefficient	0.7

3.2.3 Comparison with MCS predictions

Figure 15 shows η_r^f obtained from DEM simulations for various f_c values at $\alpha = 7$, 9, 12 and 16. The MCS-based predictions generally agree with the DEM results, confirming the validity of the proposed method. Although the MCS inputs differ—being derived from experimental measurements for $\alpha = 7$ and 9, and from DEM simulations for $\alpha = 12$ and 16—the predicted trends are consistent across all tested size ratios, indicating that the method's performance is robust to the source of size and positional information of the coarse particles. At low f_c, the MCS slightly overestimates η_r^f, due mainly to its idealized rattler identification criterion. In contrast, at high f_c the MCS tends to underestimate η_r^f, likely due to the mechanism inherent to the MCS method: a higher f_c (or equivalently, a lower fraction of coarse particles) leads to larger but fewer adjusted void circles. This mechanism is illustrated in Fig. 16 using an area-equivalent example based on adjusted void circles: a system with three voids, each accommodating up to three fine particles ($N_3 = 3$) has the same total void area as one void holding nine particles ($N_9 = 1$). When ten fine particles are distributed into these systems, the multiple-void configuration is more likely to leave some voids underfilled, producing rattlers (e.g., two in Fig. 16(a)), whereas the single large void can accommodate all particles without generating rattlers (Fig. 16(b)).

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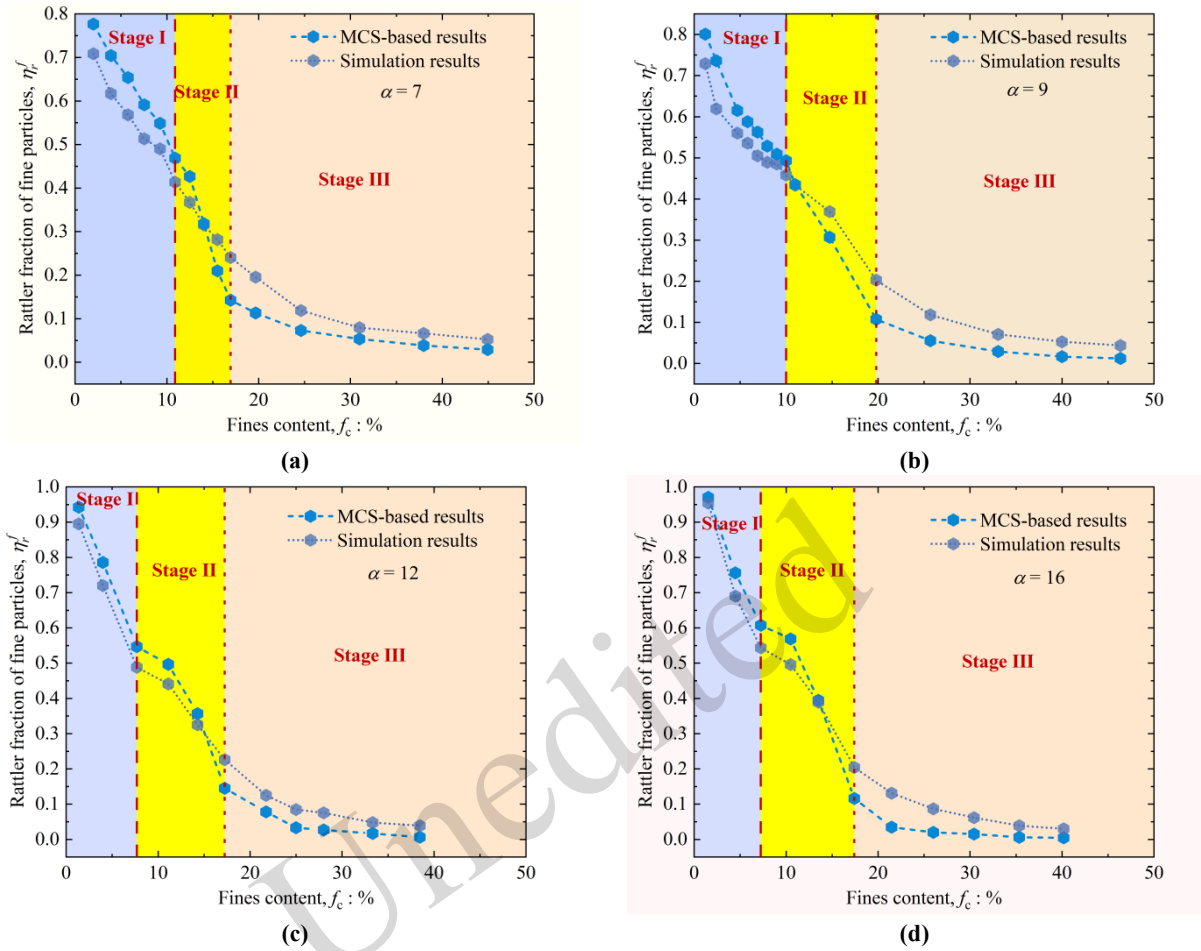

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Fig. 15 Comparison of MCS-based and simulated rattler fractions for the four size ratios (α = 7, 9, 12 and 16): (a) α = 7; (b) α = 9; (c) α = 12; (d) α = 16. Solid symbols with dashed lines represent MCS-based values and solid symbols with dotted lines represent simulated results. For α = 7 and 9, the MCS-based results are from Fig. 9, and the DEM results are from Fig. 14.

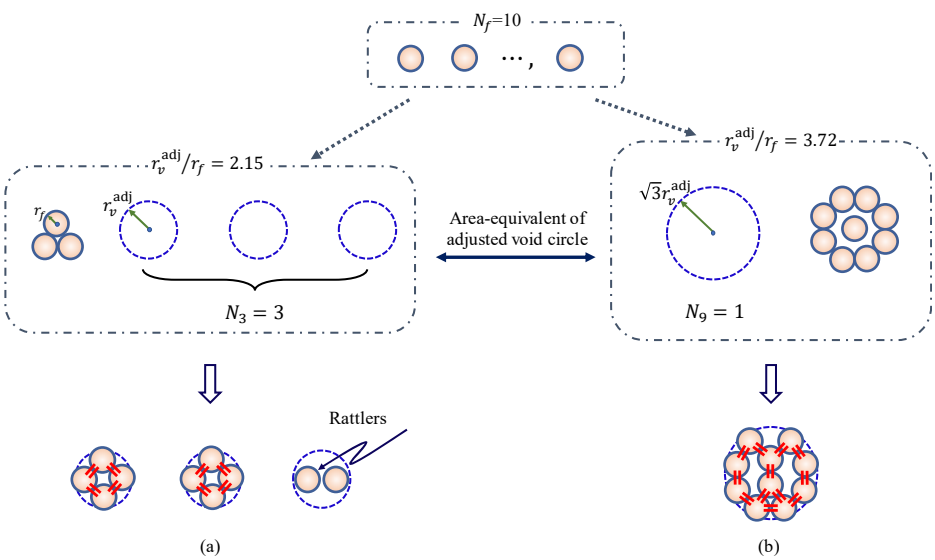

Fig. 16 Schematic of the underestimation mechanism of the MCS method at high fines content: (a) multiple small voids

may lead to underfilled voids and rattlers; (b) a single large void accommodates all particles with no rattlers, despite an equal total void area in both cases. The dashed circle represents the adjusted void circle, while short red double-solid lines denote contacts between particles and their neighbors.

In summary, at high f_c, the MCS method's idealized assumptions tend to overestimate η_r^f, while the reduced number of voids due to fewer coarse particles—despite being larger—introduces an underestimation effect. These opposing mechanisms compete, and our results suggest that the underestimation effect dominates, resulting overall in a lower MCS-predicted η_r^f compared to DEM. In contrast, at low f_c, the underestimation mechanism becomes negligible, and the overestimation due to idealized assumptions prevails.

In addition, Fig. 17 presents quantitative comparisons between DEM simulations and MCS predictions. The L2 norm (L2) remains below 0.07, the mean error (ME) below 0.06, and the maximum error (MaxE) below 0.12, indicating small deviations across all cases. Detailed definitions of the three error metrics can be found in Supplementary Materials Section 1.

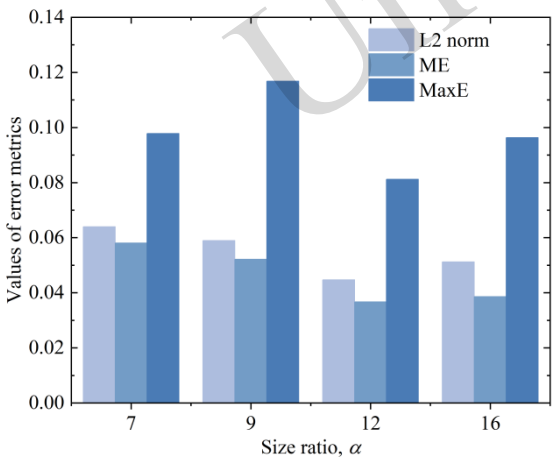

Fig. 17 Error comparison for different size ratios (α = 7, 9, 12, and 16).

4. Discussion

The proposed MCS-based approach requires the sizes and spatial positions of coarse particles as known inputs. For validation, coarse particle data were obtained from both experiments and DEM simulations in this study. Granular packings are generally generated by two approaches: dynamic methods (Cundall and Strack, 1979; Ting et al., 1993), such as DEM, which solve the equations of particle motion, and geometric methods (Bagi, 2005; Feng et al., 2003), which construct packings purely through geometric calculations. Representative geometric methods include the Inward Packing Method (Bagi, 2005) and the Advancing Front Approach (Feng et al., 2003). Compared with dynamic methods, geometric approaches are more computationally efficient and can rapidly generate large numbers of packings. However, they typically yield relatively dense configurations and face challenges in reproducing different void ratios under the same particle size distribution.

Overall, geometric methods provide a reliable means of obtaining coarse particle configurations for estimating η_r^f in dense packings. For looser systems, η_r^f may instead be approximated by fitting a functional relationship between its values in dense packings and the void ratio *e*. Although geometric methods were not directly applied in this study, they hold strong potential for extending the applicability of the MCS framework and warrant further investigation.

In addition, although the present study was restricted to 2D granular systems, the MCS-based framework is conceptually extendable to 3D packings. In this case, the void identification step can be adapted using 3D Delaunay tessellation to construct inscribed void spheres that are tangent to the four particles located at the vertices of each Delaunay tetrahedron. These inscribed spheres can then be adjusted based on the 3D maximum packing density to determine the maximum number of fine particles that can be placed within each void. The fine particle capacity in each void is directly determined from *The Best Known Packings of Equal Spheres in a Sphere* (Otto von Guericke University Magdeburg, 2025). Finally, fine particles are randomly assigned to the classified pore spheres, with their initial weights and update procedures following the same approach described in Section 2.4. The MCS is repeated multiple times to obtain statistically stable results.

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5. Conclusions

In this paper, we designed a Monte Carlo simulation (MCS)-based method for estimating the fine rattler fraction η_r^f in large-ratio binary mixtures. Its performance and potential limitations were examined by comparing predictions with experimental measurements and DEM simulations. Based on these analyses, we drew the following conclusions:

1.The MCS-based predictions closely matched the experimental results for mixtures with $\alpha = 7$ and 9, showing a slight overall overestimation. This deviation stems mainly from the idealized assumption of the maximum void capacity and is attributed partly to the contact detection criterion used in experimental image processing. At low f_c, the MCS-based predictions tend to overestimate η_r^f compared to DEM results, due mainly to its idealized identification assumptions. However, as f_c increases, the trend reverses, and η_r^f is underestimated. This is likely because the reduction in the number of adjusted void circles—resulting from a lower proportion of coarse particles—has a stronger underestimation effect than the overestimation induced by the idealized assumption, leading to an overall underprediction of η_r^f at high f_c.

2.Two transitional points in the η_r^f - f_c curve, identified by inflection points in the slope, delineate three distinct phases: (Ⅰ) a steep initial decline, (Ⅱ) a continued decline with a slight change in the slope, and (Ⅲ) a final gentle decrease. As α increases, the lower transitional fine content shifts downward, while the upper transitional content tends to shift upward.

3.Although the present study focused on 2D granular assemblies for their geometric simplicity, the developed MCS framework provides a conceptual and computational foundation for extension to more realistic 3D packings, including void identification via Delaunay tetrahedron and fine particle allocation within inscribed pore spheres.

4.The assumption of circular particles in this study simplifies the representation of granular materials. To enhance the practical relevance of the proposed methods, future work should aim to incorporate particle shape irregularities and multicomponent mixtures.

In summary, the proposed MCS method enables robust and relatively accurate estimation of the fine particle rattler fraction η_r^f using only the size and positional information of coarse particles. This framework advances both experimental analysis and theoretical modeling in granular physics and provides a foundation for extending the approach to more complex three-dimensional granular systems.

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Author contributions

Conceptualization contributed by Jing WANG and Daosheng LING; methodology by Jing WANG and Changyu SHI; formal analysis and investigation by Jing WANG and Daosheng LING; funding acquisition by Daosheng LING; supervision by Daosheng LING. The first draft of the manuscript was written by Jing WANG, and all authors read and approved the final version.

Conflict of interest

Jing WANG, Changyu SHI, and Daosheng LING declare that they have no conflict of interest.

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Electronic supplementary materials

Section S1, Table S3

中文概要

题　目：估算高粒径比二元混合物中悬浮细颗粒比例的蒙特卡洛模拟方法

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目　的： 在高粒径比二元颗粒体系中，准确估计悬浮细颗粒（fine rattler）比例对理解体系的结构与力学响应至关重要。然而，试验中通常难以直接获得颗粒间接触力信息，且细颗粒的位置和尺寸识别精度较低。本文旨在提出一种仅依赖粗颗粒尺寸与位置数据的估算方法，以解决悬浮细颗粒比例估算问题。

创新点： 1. 将悬浮细颗粒比例的估算视为不确定性量化问题，提出基于蒙特卡洛模拟（MCS）的新方法；2. 方法只需粗颗粒的尺寸与空间分布信息，无需获取接触力等其它数据；3. 在二维高粒径比体系中系统验证了方法的有效性，并通过试验与离散元（DEM）模拟对比揭示了不同细颗粒含量下的偏差规律。

方　法： 1. 利用 Delaunay 三角剖分提取粗颗粒体系的孔隙分布，并建立细颗粒填充的 MCS 框架（图 3）；2. 在多次蒙特卡洛采样中，根据孔隙容量判定细颗粒是否为悬浮颗粒，并通过统计得到平均悬浮细颗粒比例（图 6、图 7 和图 8）；3. 将 MCS 预测结果与试验观测及 DEM 模拟进行对比，评估方法的精度与适用性（图 15）。

结　论： 1. 所提出的 MCS 方法能够在无需动力学求解条件下，对悬浮细颗粒比例进行稳健且较为准确的估算；2. 研究为颗粒材料的试验分析和理论建模提供了实用框架，并展示了方法向三维复杂体系扩展的潜力。

关键词： 颗粒材料；悬浮颗粒；细颗粒含量；粒径比；DEM；蒙特卡洛

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