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

Key words: Granular materials; Rattlers; Fines content; Size ratio; Discrete element method (DEM); Monte Carlo

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Method framework

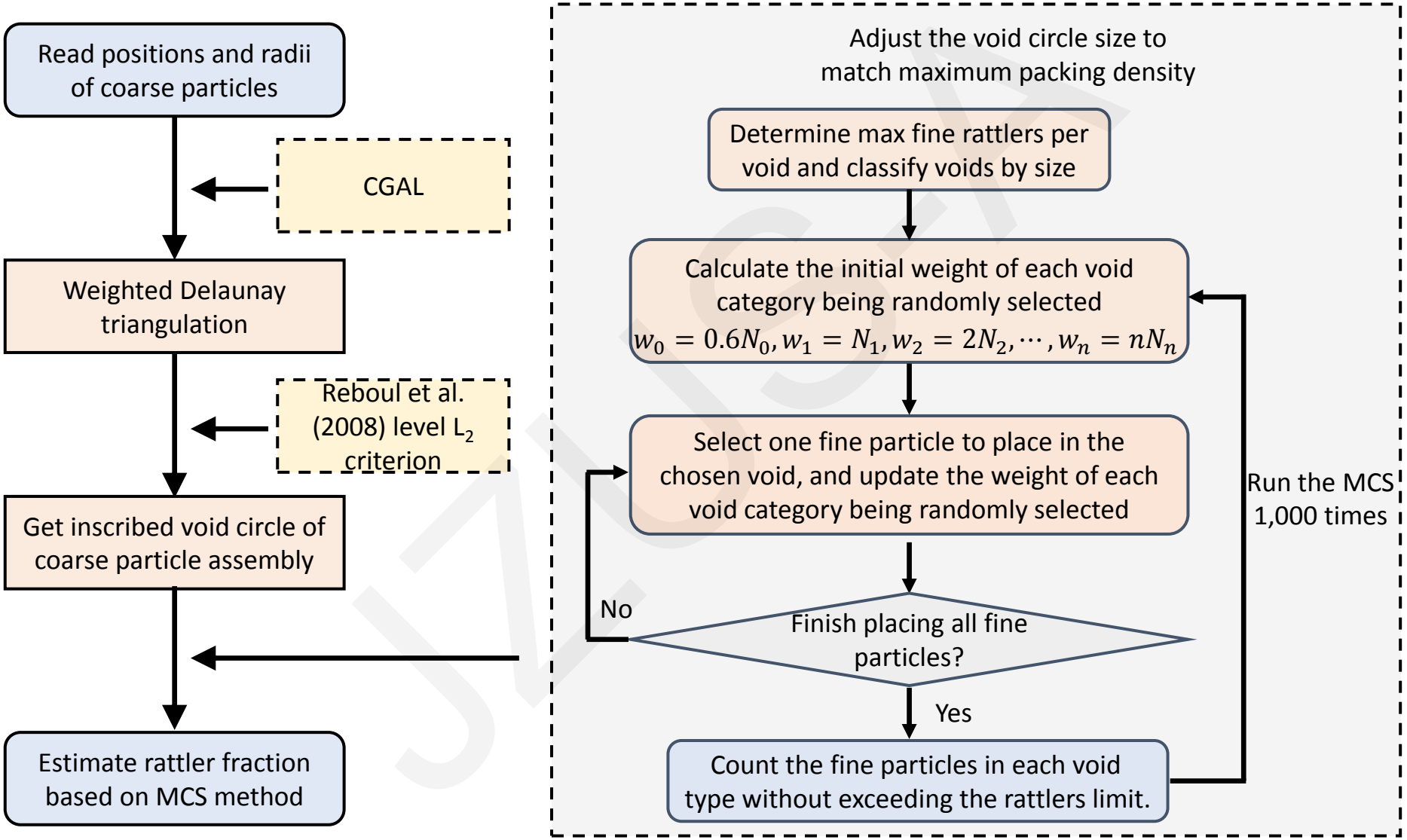
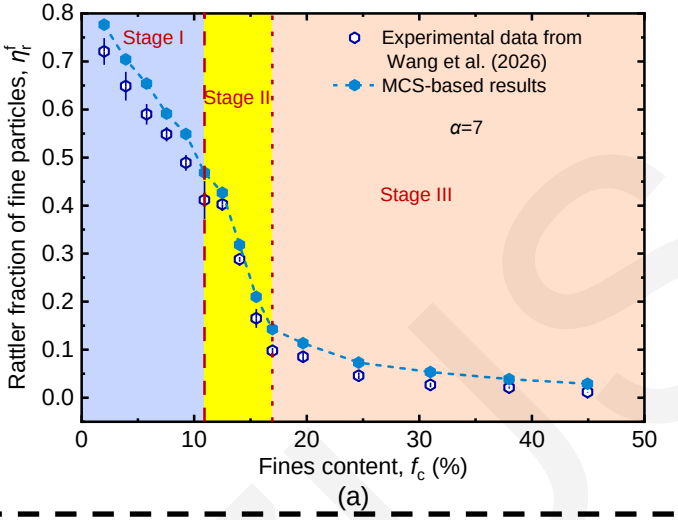


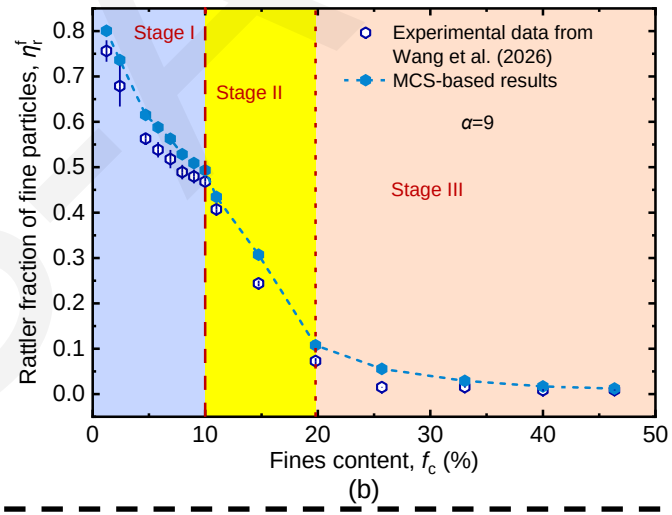
Fig. 1 Calculation procedure for the proposed MCS-based method

Results Analysis and Comparison

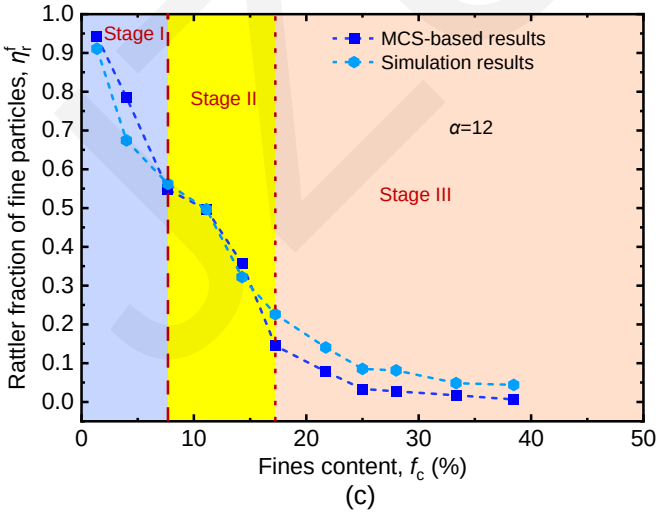
The MCS-based predictions generally agree with the experimental and DEM results

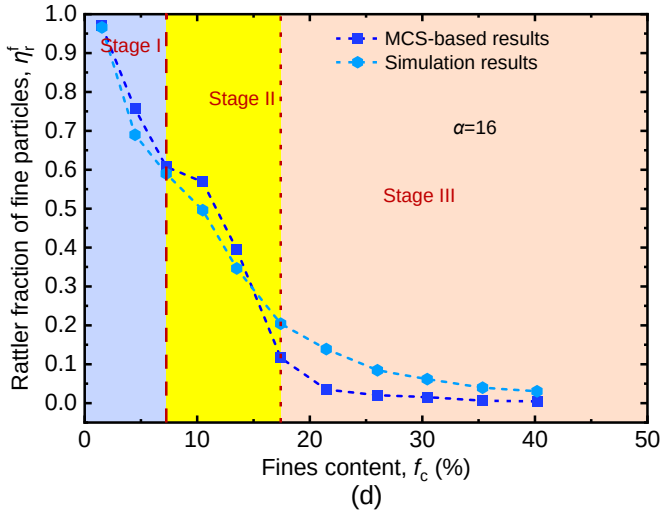
MCS prediction VS Experiments





MCS prediction VS Simulations





Results Analysis and Comparison

The L2 norm, mean error (ME), and maximum error (MaxE) between the MCS predictions and the DEM simulation results remain below 0.07, 0.06, and 0.12, respectively, indicating small deviations across all cases.

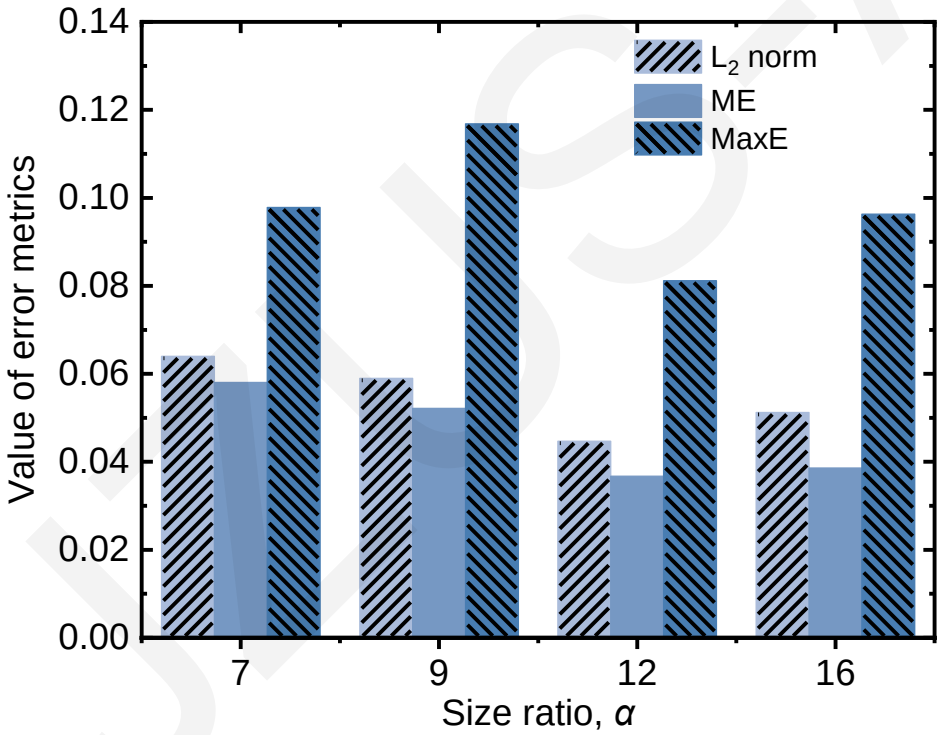


Fig. 17 Error comparison for different size ratios (α=7, 9, 12, and 16)

Main Contributions

- The proposed MCS-based method overcomes the high computational cost associated with repeated dynamic iterations in discrete element simulations.
- It enables the statistical characteristics of large samples to be accurately approximated through repeated random sampling of small-scale samples.

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Conclusions

- The MCS-based predictions closely matched the experimental results for mixtures with α=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, mainly due 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.
- 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.
- 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.