Electronic Supplementary Materials

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

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Section S1. Optimization analysis of scaling factor in MCS-based method

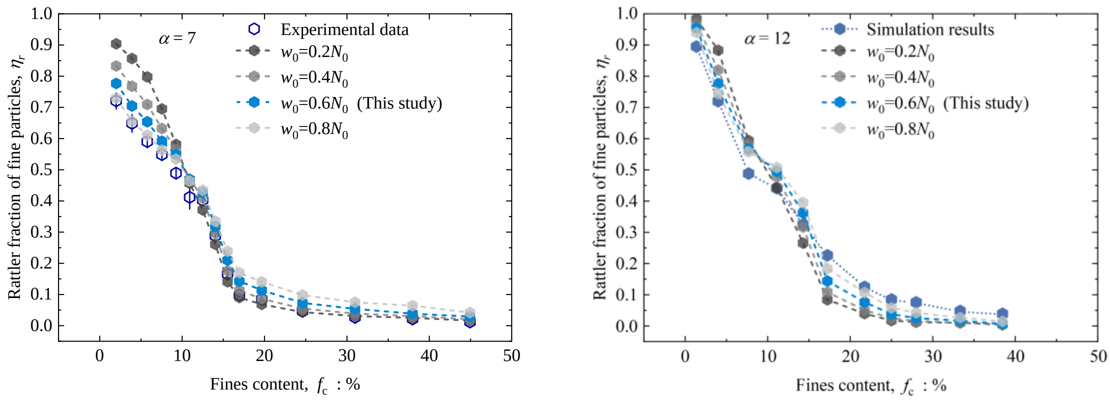
The proposed Monte Carlo Simulation (MCS)-based method includes a scaling factor ranging between 0 and 1, which is applied to the weight of the void circle N_0. Figure S1 compares the fine rattler fraction η_r^f predicted by the MCS-based method using different scaling factors for binary mixtures with size ratios α = 7 and 12. These two cases are selected to represent relatively small and large particle size ratios, respectively, within the scope of this study. To quantitatively evaluate the accuracy associated with each scaling factor, three error metrics are employed: L2 norm (L2), mean error (ME), and maximum error (MaxE), defined as follows:

$$\mathrm{L2} = \sqrt{\frac{1}{N_\mathrm{p}}\sum_{N_\mathrm{p}}\left(\eta_r^{\mathrm{pre}} - \eta_r^{\mathrm{mea}}\right)^2}, \tag{S1}$$

$$\mathrm{ME} = \frac{1}{N_\mathrm{p}}\sum_{N_\mathrm{p}}\left|\eta_r^{\mathrm{pre}} - \eta_r^{\mathrm{mea}}\right|, \tag{S2}$$

$$\mathrm{MaxE} = \max\left(\left|\eta_r^{\mathrm{pre}} - \eta_r^{\mathrm{mea}}\right|\right). \tag{S3}$$

Here, η_r^{pre} denotes the fine rattler fraction predicted by the MCS-based method, η_r^{mea} refers to the corresponding measured value, either from experiments for α = 7 or DEM simulations for α = 12, and N_p is the total number of data points considered for comparison.



(a) (b)

Fig. S1. Comparison of fine rattler fraction predicted by the MCS-based method under different void size scaling factors for binary mixtures with size ratios α = 7 and 12: (a) α = 7; (b) α = 12

Tables S1 and S2 report the values of the three error metrics across a range of scaling factors for α = 7 and 12, respectively. Based on these comparisons, a scaling factor of 0.6 is adopted throughout this study. This value consistently provides a favorable balance among the three error measures, offering sufficiently accurate and robust predictions of the fine rattler fraction across different fines contents and particle size ratios.

Table S1. Error metrics for estimated fine rattler fraction at different values of factor for size ratio α = 7

Factor	L2 norm	mean error	maximum error
0.2	0.1015	0.0523	0.2078
0.4	0.0622	0.0432	0.1192
0.6	0.0426	0.0397	0.0637
0.8	0.0447	0.0399	0.0731

Table S2. Error metrics for estimated fine rattler fraction at different values of factor for size ratio α = 12

Factor	L2 norm	mean error	maximum error
0.2	0.0894	0.0120	0.1632
0.4	0.0702	0.0082	0.1181
0.6	0.0547	0.0007	0.0825
0.8	0.0444	0.0010	0.0700

Section S2. Numerical simulation cases

Table S3 DEM simulation cases for different size ratios

Simulation No.	Size ratio α (coarse/fine)	Fines content f_c (%)	Number of particles
1	7	2.00	4172
2		3.92	6135
3		5.77	8022
4		7.55	10463
5		9.26	12324
6		10.91	14161
7		12.50	16820
8		14.04	18591
9		15.52	20301
10		16.95	21952
11		19.67	7883
12		24.62	10183
13		30.99	17066
14		37.97	18383
15		44.94	22837
16	9	1.22	4382
17		2.41	7126
18		4.71	6218
19		5.81	7956
20		6.90	9617
21		7.95	11818
22		8.99	32301
23		10.00	15717
24		10.99	41419
25		14.74	7815
26		19.80	14406
27		25.69	25433
28		33.06	27921
29		40.00	35420
30		46.36	39121
31	12	1.37	3348
32		4.00	8384
33		7.69	14972
34		11.11	19114
35		14.29	22628
36		17.24	26898
37		21.74	32773
38		25.00	37537
39		28.00	37622
40		33.33	44614
41		38.46	57199
42	16	1.54	12536
43		4.48	27791
44		7.25	37975
45		10.49	19003
46		13.51	24436
47		17.42	33110
48		21.47	41251

49	26.01	48230
50	30.43	66331
51	35.35	73441
52	40.19	72474