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1 **Validation of a stochastic digital packing algorithm** 2 **for porosity prediction in fluvial gravel deposits**

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10 **Abstract**

11 Porosity as one of the key properties of sediment mixtures is poorly
12 understood. Most of the existing porosity predictors based upon grain size
13 characteristics have been unable to produce satisfying results for fluvial
14 sediment porosity, due to the lack of consideration of other porosity-
15 controlling factors like grain shape and depositional condition. Considering
16 this, a stochastic digital packing algorithm was applied in this work, which
17 provides an innovative way to pack particles of arbitrary shapes and sizes
18 based on digitization of both particles and packing space. The purpose was
19 to test the applicability of this packing algorithm in predicting fluvial
20 sediment porosity by comparing its predictions with outcomes obtained
21 from laboratory measurements. Laboratory samples examined were two
22 natural fluvial sediments from the Rhine River and Kall River (Germany),
23 and commercial glass beads (spheres). All samples were artificially
24 combined into seven grain size distributions: four unimodal distributions
25 and three bimodal distributions. Our study demonstrates that apart from
26 grain size, grain shape also has a clear impact on porosity. The stochastic
27 digital packing algorithm successfully reproduced the measured variations
28 in porosity for the three different particle sources. However, the packing
29 algorithm systematically overpredicted the porosity measured in random

30 dense packing conditions, mainly because the random motion of particles
31 during settling introduced unwanted kinematic sorting and shape effects.
32 The results suggest that the packing algorithm produces loose packing
33 structures, and is useful for trend analysis of packing porosity.

34 **Keywords:** Porosity; Sediment; Grain shape; Random packing; Rivers

35 **1. Introduction**

36 Porosity prediction of sedimentary deposits is of interest in a fluvial
37 environment. Previous studies have shown that porosity, as a key structural
38 property, plays an important role in the morphological, ecological and
39 geological characteristics of fluvial systems. Morphologically, porosity
40 governs the initiation of sediment motion and bank collapse (e.g., Wilcock,
41 1998; Vollmer and Kleinhans, 2007). Ecologically, porosity determines the
42 interstitial space of the hyporheic zone for aquatic habitats (e.g., Boulton et
43 al., 1998). Geologically, porosity dominates the exploitable reserve of oil,
44 gas, and groundwater stored in the voids of fluvial deposits (e.g., Athy,
45 1930). To date, existing porosity predictors can generally be classified into
46 two types: (1) empirical predictors; and (2) theoretical predictors. Most
47 efforts to predict porosity have been empirically driven, to a large extent
48 based upon median grain size D_{50} (e.g., Carling and Reader, 1982; Wu and
49 Wang, 2006), sorting coefficient σ (e.g., Wooster et al., 2008), or a
50 combination of different grain size characteristics (e.g., Frings et al., 2011;
51 Desmond and Weeks, 2014). Theoretical predictors such as geometrical
52 models (e.g., Ouchiyama and Tanaka, 1984; Suzuki and Oshima, 1985) or
53 analytical models (e.g., Yu and Standish, 1991; Koltermann and Gorelick,
54 1995; Esselburn et al., 2011) relate porosity to the full grain size distribution

55 of perfect spheres. The performance of these predictors has been
56 investigated by comparing porosity values measured in situ with those
57 computed by the predictors (e.g., Frings et al., 2008, 2011). Unfortunately,
58 these predictors produced unsatisfying results in predicting fluvial sediment
59 porosity (Frings et al., 2011), probably because such predictors mainly
60 focused on grain size characteristics, ignoring other porosity-controlling
61 factors such as depositional environment and grain shape.

62 Effects of grain shape on porosity have received less attention, due to
63 the complexity of arbitrary shapes of natural particles. Over the past decade,
64 the application of computer simulations for the study of granular particle
65 packings has become more popular, supported by developments in the
66 computer hardware industry. However, most of the computer simulations
67 have been limited to simple analytical geometries such as cylinders (Zhang
68 et al., 2006), disks (Desmond and Weeks, 2009), ellipsoids (Donev et al.,
69 2007; Zhou et al., 2011) and spherocylinders (Abreu et al., 2003; Williams
70 and Philipse, 2003; Zhao et al., 2012). The major reason is the practical
71 difficulty of representing and handling irregular shapes using vector-based
72 approaches. Traditional ways to construct an irregular particle require the
73 user to place spherical elements within a meshed polyhedral body (e.g.,
74 Wang et al., 2007; Matsushima et al., 2009; Ferrellec and McDowell, 2010;
75 Fukuoka et al., 2013), which consumes high computational costs with large
76 numbers of components (spheres) involved (Hubbard, 1996; Song et al.,
77 2006). Although techniques using 3D polyhedral (Latham et al., 2001) or
78 continuous superquadric functions (Williams and Pentland, 1992; Lu et al.,
79 2012) provide a straightforward way to generate irregular particle shapes,

80 complex contact-detection algorithms are needed, leading to deterioration in
81 simulation speed as particle complexity increases (Johnson et al., 2004).

82 In order to overcome these difficulties, a stochastic digital packing
83 algorithm was developed (Jia and Williams, 2001). The packing algorithm
84 is distinguished from the traditional vector-based packing models by
85 digitization of both particles and packing space, allowing for a much easier
86 and computationally efficient way to pack particles of irregular shapes with
87 no more than an ordinary PC. These advantages make it attractive to create
88 packings of complex fluvial deposits, and to study the grain shape effects on
89 porosity. Applications of this stochastic digital packing algorithm have
90 proven to provide relatively accurate porosity predictions for both fine
91 powders (Jia et al., 2007) and large spheres (Caulkin et al., 2006, 2007) in
92 the fields of material science and engineering chemistry. Nevertheless, the
93 packing algorithm has not yet been used for generating packings of fluvial
94 deposits. Therefore, the primary purpose of this work was to test the
95 applicability of the stochastic digital packing algorithm in predicting fluvial
96 sediment porosities. In this study, we focused on fluvial gravel mixtures and
97 did so by comparing the predicted porosities with those obtained from
98 laboratory measurements.

99 **2. Materials and methods**

100 2.1. Particle acquisition and analysis

101 The particles employed for this study came from three different sources:
102 (1) fluvial gravels from the Rhine River (Germany), (2) fluvial gravels from
103 the Kall River (Germany), and (3) commercial glass beads. The Rhine
104 sediments were collected from the channel bed between the barrage of

105 Iffezheim and the German-Dutch border between July 2008 and April 2011.
106 Quartz is the dominant lithology. The Kall sediments were collected from
107 the channel bed near the river mouth in June 2014. Slate is the dominant
108 lithology.

109 After acquisition, the fluvial sediments were carefully cleaned by
110 flushing with fresh water, dried in an oven at 105 °C for 48 h and sieved
111 into seven size fractions: 2.8-4 mm, 4-5.6 mm, 5.6-8 mm, 8-11.2 mm, 11.2-
112 16 mm, 16-22.4 mm, 22.4-31.5 mm. Subsequently, these fractions were
113 combined into seven grain size distributions: four unimodal ones with
114 logarithmic standard deviations (σ_ϕ) of 0.00, 0.32, 0.49 and 0.71, and three
115 bimodal ones, with the finer mode, making up either k=30, k=50 or k=70
116 percent of the distribution (Fig. 1). The glass beads with seven size fractions
117 of 3, 4, 6, 8, 11, 16 and 22 mm were also combined into the same
118 distributions as above.

119 For the fluvial sediments, nine representative particles were chosen
120 based on visual judgments from each of the seven sieve fractions, and
121 digitized (Fig. 2) using a nonmedical X-ray computed tomography (CT)
122 scanner. Shape analysis was done according to the classic Zingg diagram
123 (Zingg, 1935), which categorizes particle shape into sphere, disc, blade and
124 rod categories on the basis of the elongation ratio (b/a) and flatness ratio
125 (c/b), where a, b and c are the long, intermediate and short orthogonal axes
126 respectively of the smallest volume imaginary box that can contain the
127 particle (Blott and Pye, 2008). It can be seen in Figure 3 that most of the
128 Rhine sediments locate within the sphere area while the Kall sediments are
129 dominated by disks and blades. According to Krumbein's (1941) equation

130 (1), the intercept sphericity (ψ) for each selected particle was calculated,
131 with an average intercept sphericity of 0.74 gained for the Rhine sediments
132 and 0.55 for the Kall sediments.

$$133 \quad \psi = \sqrt[3]{\frac{b*c}{a^2}} \quad (1)$$

134 2.2. Laboratory porosity measurements

135 The water displacement method (Bear, 1972) was used for porosity
136 measurements. The experimental procedure was as follows: firstly, a plastic
137 cylinder with an inner diameter of 104 mm was partially filled with a known
138 volume of water V_w larger than the expected pore volume of the particles to
139 be added. Then, particles of 3 kg mass were added into the cylinder in small
140 well-mixed portions, together with gently tapping the side of the cylinder in
141 order to dislodge trapped air bubbles and obtain a stable, dense packing. The
142 final water level was visually read to obtain the whole accumulated volume
143 V_a ($V_a = V_w + V_s$, where V_s is the volume of the solid fraction). The jagged
144 surface of the particle packing caused by the wide range of sizes and shapes
145 was then smoothed by hand and the total volume of the particle packing V_t
146 (including pores) was obtained through reading the height of the particle
147 packing. Eventually, the porosity was computed as $n = V_p/V_t$, where V_p
148 ($= V_t - (V_a - V_w)$) is the pore volume of the particle packing.

149 In total, 42 laboratory porosity experiments were performed as a basis
150 for the validation of the stochastic digital packing algorithm: 14 experiments
151 with the sub-spherical Rhine sediments (7 distributions, each two times), 14
152 experiments with low-sphericity Kall sediments (again 7×2) and 14
153 experiments with the spherical glass beads (again 7×2).

154 2.3. Porosity simulation

155 The stochastic digital packing algorithm of Jia and Williams (2001) is
156 designed to pack particles of arbitrary sizes and shapes in a confined space
157 of arbitrary geometry. In this packing algorithm, every element is digitized:
158 each particle as a coherent collection of voxels, the packing space (in a
159 container) as a lattice grid, and the movements take place in units of grid
160 cells. During the simulation, the movements of particles, both translational
161 and rotational, are random. In 3D, there are 26 possible translational
162 directions: 6 orthogonal and 20 diagonal. The diagonal moves are treated as
163 a combination of two orthogonal moves. To ensure particles settle while still
164 make use of every available space, a rebounding probability is used. An
165 upward movement (which may be an orthogonal move or part of a diagonal
166 move) is only realized with this probability. After translation, a trial rotation
167 follows, and it is accepted if the rotation does not result in overlaps.
168 Compared with vector-based approaches and for complex shapes, this
169 digital approach is advantageous in several respects. First, there is no
170 conversion or parameterization required, since objects digitized by modern
171 imaging devices, such as X-ray tomography (e.g., Richard et al., 2003) or
172 nuclear magnetic resonance imaging (e.g., Kleinhans et al., 2008), are
173 already in the digital volumetric format required by the packing algorithm.
174 Secondly, collision and overlap detection (normally the most
175 computationally expensive part of packing simulations) is much easier to
176 implement as computer code, and usually faster to execute for complex
177 shapes. Thirdly, the number of voxels used to represent objects, and hence
178 to a large extent the simulation runtime, does not necessarily increase with

179 shape complexity. The reverse is also true: it does not necessarily reduce
180 with shape simplification either. Further details on the stochastic digital
181 packing algorithm can be found elsewhere (Jia and Williams, 2001; Caulkin
182 et al., 2006, 2007).

183 In order to produce porosity results comparable to those aforementioned
184 measurements, simulation conditions need to be set up to resemble the
185 laboratory experiments, with respect to the packing space, the particle
186 mixtures and the packing process. The digital objects (i.e., packing space
187 and particles) were prepared with DigiUtility, which is a bundled tool for
188 viewing, manipulating and preparing digital files for this packing algorithm.
189 In DigiUtility, a cylinder (packing space) with solid boundary was built with
190 the size of 104 mm in diameter, and 300 mm in height, which is slightly
191 higher than the largest real packing heights (about 250 mm) to ensure all the
192 particles would drop into it. The particle mixtures (i.e., number of particles
193 in each of the fractions) employed in these simulations were derived on a
194 weight-to-weight basis. For glass beads, the numbers of particles in each
195 fraction were determined as the ratio of the real mass of each fraction to the
196 single particle mass (density of 2500 kg/m^3 used for glass beads). The
197 regular spherical shapes with different sizes were directly created in digital
198 formats using DigiUtility. In the case of the fluvial sediments, we used nine
199 digitized typical particles to represent each fraction and repeated them as
200 many times as needed to make up the feedstock according to the required
201 grain size distributions. The density of fluvial gravels was set to 2650 kg/m^3 .
202 Resolution of 0.5 mm/voxel for the digital objects was assigned as it offers

203 relatively precise representation of the real particles in both dimension and
204 shape, and also limits the computational cost to a feasible amount.

205 Having the digital objects created, a range of options and parameters
206 was set to mimic the packing process. The source was set to “rain-dropping”
207 mode to let the particles randomly drop from a circular area above the
208 cylinder. In addition to the translational movements, particles were also
209 allowed to rotate randomly during the simulation. Optimized values of the
210 parameters (rebounding probability, addition rate and number of time steps)
211 that control the generated packing structures were chosen such as to create
212 the densest possible packings. By doing so, simulation conditions (Table 1)
213 matched the experimental setups as close as possible. Finally, the porosity
214 of the digital packings was determined as the ratio of the number of empty
215 voxels to the total number of voxels within the corresponding packing space.
216 Porosity was calculated for the lower 90% of the mixture to exclude effects
217 of surface irregularities. Each simulation was also done twice and 42
218 simulations were achieved in total.

219 **3. Results**

220 3.1. Measured porosity

221 The porosity measured in the laboratory experiments is shown in Figure
222 4. For the unimodal particle mixtures, porosity decreases with increasing
223 logarithmic standard deviations, while the bimodal particle mixtures
224 generally have lower porosity than the unimodal mixtures. This variation in
225 porosity reflects the mixing effect between small and large particles.

226 Porosity comparisons between the three different particle sources show
227 the low-spherical Kall sediments and the spherical glass beads produced

228 higher porosity than the sub-spherical Rhine sediments, which confirms that
229 there is a decrease and then increase in porosity as particle shape varies
230 from spherical to platy (Tickell and Hiatt, 1938; Zou and Yu, 1996). On the
231 other hand, in the case of the bimodal particle mixtures, different tendencies
232 toward the porosity are appreciable (Fig. 4B), suggesting grain shape exerts
233 a quite complicated influence on porosity, not merely in variation of amount
234 but in variation of trend.

235 It should be noted that the dense sediment deposits packed by hand in
236 the laboratory experiments are not fully representative of natural situations
237 where grain arrangement is determined by depositional conditions, such as
238 flow impact (with near-bed turbulence playing an important role) and burial
239 depth (compaction mechanism). This topic is beyond the current effort.
240 Nonetheless, based on the comparisons between field measurements of
241 porosity in the River Rhine (28 measurements on the channel bed and 18
242 measurements on the river banks, focusing on subsurface sediments) and
243 measurements in the laboratory (Frings et al., 2011), it was found that in
244 most cases (59%), the difference between is less than 0.03 (Fig. 5), with an
245 average porosity of 0.24 obtained *ex situ* and 0.22 *in situ*.

246 3.2. Algorithm behavior

247 The behavior of the stochastic digital packing algorithm is presented in
248 Figure 6. In order to validate the packing algorithm, comparisons were made
249 between the measured and simulated porosity outcomes. Figure 7 clearly
250 shows that the packing algorithm successfully captures the measured
251 variation in porosity due to grain size distributions for each particle source.
252 While the packing algorithm also seems to be able to mimic the measured

253 variation due to grain shape for a given grain size distribution, providing
254 that the glass beads (spheres) are not taken into account (Fig. 8).

255 However, nearly all simulated porosities were systematically
256 overestimated compared to the experimental measurements. To easily
257 recognize these discrepancies, relative errors between the measured and
258 simulated porosities were calculated (Table 2). The average relative error is
259 29.4% for the Rhine sediments, 21.7% for the Kall sediments and 6.6% for
260 the glass beads, indicating that the packing algorithm predicted relatively
261 higher porosities when it comes to fluvial sediments with irregular shapes.
262 Figure 9 shows the comparison between these discrepancies over the seven
263 grain size distributions. For the unimodal particle mixtures, the
264 discrepancies are growing as logarithmic standard deviation increases (Fig.
265 9A). For the bimodal particle mixtures, with the finer mode increasing from
266 30% to 70%, the discrepancies for fluvial sediments decrease while the
267 discrepancies for glass beads increase (Fig. 9B).

268 **4. Discussion**

269 The purpose of determining the porosities of the samples was twofold:
270 first, to point out that apart from grain size, grain shape also has a clear
271 impact on porosity (shown in section 3.1), and second, to serve as a basis of
272 comparison for the porosities predicted from the stochastic digital packing
273 algorithm. It is shown in section 3.2 that although the packing algorithm is
274 able to follow the experimental trend, systematic overestimation of the
275 porosity is noticeable, especially for the fluvial sediments. The remarkable
276 discrepancies between can be caused by (1) measurement inaccuracies,
277 and/or (2) simulation inaccuracies.

278 4.1. Measurement inaccuracies

279 For the laboratory measurements, the reading errors related to the water
280 levels and packing heights dominate the accuracy of outputs. The water
281 levels were visually read to obtain the whole accumulated volumes V_a with
282 a deviation of about 1 mm, and readings of the packing heights for gaining
283 the total volume of particle packing V_t (including pores) were achieved with
284 an accuracy of ~3 mm. These inevitable reading errors can lead to the
285 absolute error of the porosity to be ~0.01 for the measurements. However,
286 measured inaccuracies are small compared to the apparent differences
287 between the measured and simulated porosities, particularly for fluvial
288 sediments.

289 4.2. Simulation inaccuracies

290 4.2.1. Digitization inaccuracy

291 As can be seen in Figure 10, the arrangements of particles leave
292 unexpected pore spaces. One reason for this may be the digitization errors of
293 digital objects represented at a resolution of 0.5 mm/voxel. The effect can
294 be supported by the fact that the porosity of 0.355 simulated for glass beads
295 is less than the limit of 0.36 in a random dense packing of spheres (Scott,
296 1960; Allen, 1985; Yu and Standish, 1991; Weltje and Alberts, 2011). This
297 is probably because the spherical shape of glass beads is not perfectly
298 described at such a resolution (0.9% digitization error), causing a reduction
299 of porosity. Korte and Brouwers (2013) also observed the same effects in
300 the simulation of packing 3D digitalized spheres under different resolutions.
301 For this reason, a test for the ID 5 case (Table 2) was carried out with a
302 higher resolution of 0.25 mm/voxel to decrease the digitized errors,

303 especially for smaller particles. This gave a slightly lower porosity of 0.37
304 instead of 0.38 at 0.5 mm/voxel resolution, indicating that effects of
305 digitization errors are not too significant when compared to the
306 discrepancies between measured and simulated porosities.

307 Another error arises from the strict non-overlap requirement in the
308 algorithm. Imagine two large objects side by side. If for any reason, there is
309 a voxel protruded from either of the objects, this single voxel can stop the
310 two objects from coming closer, thus leaving a large gap. In reality or in
311 DigiDEM simulations, where forces instead of probabilities are used to
312 determine in which direction and by how much each object moves in the
313 next time step, this would not have happened.

314 4.2.2. Process control parameters

315 Another cause of simulation inaccuracy is the settings of process control
316 parameters that affect the simulated packing structures, which are
317 rebounding probability, addition rate and number of time steps. We did a
318 sensitivity analysis to define the effects of these parameters on porosity.
319 This was done by running a number of simulations in which one of the
320 parameters was varied while keeping the others constant. To perform these
321 simulations, 750 spherical particles (6.4 mm in diameter) and a cylinder
322 (64mm in both diameter and height) were used. Resolution was set to 0.4
323 mm/voxel, giving a slight difference (<1% digitization error) between the
324 digital volumes and real volumes.

325 Rebounding probability, designed to allow particles to move upwards,
326 provides a non-physical way to generate vertical vibrations. The original
327 intention of having a rebounding probability is to make it possible for

328 particles to escape from their cramped places and continue to explore more
329 suitable space to fit in, thereby simulating sediment compaction. The
330 rebounding probability can be set between 0 and 1. A value of 0 means no
331 rebounding and hence no vertical vibration applied. A value of 1 means
332 particles having the same probability to move up or down, and hence kept
333 suspended. To investigate its effects on porosity, seven rebounding
334 probabilities varying from 0.1 to 0.7 were tested, while the addition rate and
335 number of time steps remained the same (Table 3). The sensitivity analysis
336 shows that bulk porosities vary parabolically as a function of the rebounding
337 probability (Fig. 11A). The lowest porosity values appear at rebounding
338 probabilities of 0.3-0.5, while lower and higher rebounding probabilities
339 give higher porosities.

340 Addition rate controls the speed of introduction of particles into the
341 packing space. Simulations with seven fixed addition rates were performed
342 with the same sets of rebounding probability, and number of time steps
343 (Table 4). Slower addition rates tend to generate denser packing structures,
344 with bulk porosities decreasing from 0.46 to 0.42 (Fig. 11B). This effect is
345 because with slower addition rates, particles have more time to find a better
346 fitting position before being locked-in by new additions, resulting in denser
347 packing structures.

348 In the packing algorithm, three types of time steps are defined: normal
349 time steps, extra time steps and wind up time steps. Normal time steps are
350 those during which particles drop into the packing space. They are closely
351 related to the addition rate. For example, if the addition rate is chosen such
352 that one particle drops down every 10 time steps, 1000 normal time steps

353 are needed to introduce 100 particles into the packing space. In the case that
354 a previously introduced particle still remains on top of the container, the
355 next particle might be prevented from being introduced. In this instance, the
356 next particle has to “wait” and extra time steps are needed to finish the
357 packing. Wind up time steps are time steps at the end of a simulation during
358 which no more particles are added and the rebounding probability is set to
359 zero. These time steps enable the whole packing structure to consolidate.
360 During the sensitivity analysis, only the effect of wind up time steps on
361 porosity was assessed, since the effect of normal and extra time steps is
362 directly related to the addition rate. The number of wind up time steps was
363 varied between 0 and 32000 (Table 5), and shows no systematic effect on
364 porosity (Fig. 11C).

365 The sensitivity analysis confirms that the settings we chose for the
366 validation of the stochastic digital packing algorithm (Table 1) result in the
367 densest possible packings. This shows that the overestimation of porosity by
368 this packing algorithm cannot be solved by choosing different settings for
369 the simulations.

370 4.2.3. Random walk-based algorithm

371 The reasons why the simulations failed to yield random dense packing
372 structures can be explored in the random walk-based packing algorithm, by
373 which the translational and rotational movements of particles during the
374 simulation are completely random. Looking at the cross sections of the
375 digital packings (Fig. 10) closely, the mixing of the particles is not uniform
376 as smaller particles are more likely to concentrate at the bottom layer,
377 particularly for the bimodal distributions with percentage of small particles

378 increasing from 30% up to 70%. The phenomenon can be interpreted by
379 kinematic sorting (i.e., segregation) effects. This is because particles kept
380 moving randomly throughout the simulation, thus giving more chances for
381 smaller particles to move through the pore spaces between larger particles
382 and reach the bottom layer. Observations from Figure 10 also suggest that
383 shape effects strongly affect the simulated packing structures of fluvial
384 sediments compared to the packings of glass beads. Because of random
385 rotational motions during the simulation, the arrangements of particles with
386 irregular shapes lead to create larger voids, especially between larger
387 particles. For the simulations of glass beads, shape effects are
388 inconsequential because the rotation of a sphere has no impact on particle
389 packing. Therefore, kinematic sorting can fully explain the growing
390 discrepancy trend for glass beads over the seven grain size distributions,
391 while shape effects are the dominant reason that causes the porosity to be
392 significantly overestimated for fluvial sediments (Fig. 9).

393 **5. Conclusions**

394 The applicability of a stochastic digital packing algorithm in predicting
395 porosity of fluvial gravel deposits was validated. The conclusions are
396 summarized as follows: (1) Apart from grain size, grain shape has a clear
397 impact on porosity. (2) The packing algorithm provides an innovative way
398 to simulate fluvial sediment mixtures with arbitrary shapes. (3) The packing
399 algorithm correctly reflects the mixing effect on porosity for unimodal
400 particle mixtures and also reproduces the differences in porosity for bimodal
401 particle mixtures. However, in all cases, the packing algorithm
402 systematically overestimates porosity mainly due to the unwanted kinematic

403 sorting effects as well as shape effects introduced by the random motion of
404 particles. (4) The packing algorithm is useful for trend analysis of packing
405 porosity; but for a quantitative match a more rigorous model such as
406 Discrete Element Method (DEM) where particle motion is physics-based
407 may be needed.

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547 **Figure captions**

548 **Fig. 1.** Four unimodal (A, B, C, D) and three bimodal (E, F, G) grain size
549 distributions used for the porosity measurements and simulations.

550 **Fig. 2.** Nine representative digitized particles in the 22.4-31.5 mm fraction
551 of (A) Rhine sediments, and (B) Kall sediments, represented at a resolution
552 of 0.5 mm/voxel.

553 **Fig. 3.** Shape properties of (A) Rhine sediments, and (B) Kall sediments in
554 the Zingg classification. ($n = 9 \times 7 = 63$)

555 **Fig. 4.** Measured porosity for the Rhine sediments, Kall sediments and glass
556 beads over the four unimodal distributions represented by logarithmic
557 standard deviation (A) and three bimodal distributions represented by
558 percentage of fine mode (B).

559 **Fig. 5.** Porosity difference between field measurements and laboratory
560 measurements, based on the porosity data set provided by Frings et al.
561 (2011). The study area was the 520 km long river reach between the barrage
562 of Iffezheim (Rhine kilometer 334) and the German-Dutch border (Rhine
563 kilometer 865).

564 **Fig. 6.** Generated digital packings for (A) Rhine sediments, (B) Kall
565 sediments, and (C) glass beads. From left to right, the packings represent the
566 four unimodal distributions (1, 3, 5, 7 fractions), and three bimodal
567 distributions (30%, 50%, 70% proportion of fine mode).

568 **Fig. 7.** Comparison of model predictions with experimental data for each
569 particle source over the four unimodal distributions (A, C, E) and three
570 bimodal distributions (B, D, F).

571 **Fig. 8.** Comparison of model predictions with experimental data between
572 the three different particle sources (i.e., the spherical glass beads, the sub-
573 spherical Rhine sediments and the low-spherical Kall sediments) for a given
574 grain size distribution. A to G represents the four unimodal distributions (1,
575 3, 5, 7 fractions), and three bimodal distributions (30%, 50%, 70%
576 percentage of fine mode).

577 **Fig. 9.** Comparisons between relative errors over the four unimodal
578 distributions (A), and three bimodal distributions (B).

579 **Fig. 10.** Cross section images of the generated digital packings for (A)
580 Rhine sediments, (B) Kall sediments, and (C) glass beads. From left to right,
581 the packings represent the four unimodal distributions (1, 3, 5, 7 fractions),
582 and three bimodal distributions (30%, 50%, 70% percentage of fine mode).

583 **Fig. 11.** Sensitivity analysis of process control parameters on porosity,
584 including (A) Rebounding probability, (B) Addition rate, and (C) Windup
585 timesteps. Each simulation was conducted three times and the error bar
586 shows 95% confidence interval for the simulated porosities.

587

Table 1. Set-up conditions applied in simulations

Parameters	Values
Resolution	0.5 mm/voxel
Container diameter	104 mm
Dropping height	300 mm
Sediment density	2650 kg/m ³
Glass density	2500 kg/m ³
Adding source	Rain-dropping mode
Rotation	Complete random
Rebounding probability	0.35
Addition rate	1 particle/every 50 timesteps
Windup timesteps	2000

588

Table 2. Porosity outcomes attained from laboratory measurements and simulations (a, standard deviation; b

ID	Description of grain size distribution	Laboratory Measurements					
		1 [#]	2 [#]	Mean	SD ^a		
1	1 Fraction	0.370	0.372	0.371	0.001		
2	Rhine sediments	Unimodal distributions	3 Fractions	0.359	0.353	0.356	0.003
3		5 Fractions	0.346	0.342	0.344	0.002	
4		7 Fractions	0.317	0.313	0.315	0.002	
5		30% ^b	0.272	0.267	0.270	0.003	
6	Bimodal distributions	50% ^b	0.284	0.294	0.289	0.005	
7		70% ^b	0.300	0.297	0.299	0.002	
8		1 Fraction	0.383	0.380	0.382	0.002	
9	Kall sediments	Unimodal distributions	3 Fractions	0.385	0.380	0.383	0.003
10		5 Fractions	0.368	0.364	0.366	0.002	
11		7 Fractions	0.331	0.324	0.328	0.004	
12		30% ^b	0.325	0.315	0.320	0.005	
13	Bimodal distributions	50% ^b	0.316	0.317	0.317	0.001	
14		70% ^b	0.314	0.312	0.313	0.001	
15	1 Fraction	0.365	0.362	0.364	0.002		
16	Glass beads	Unimodal distributions	3 Fractions	0.383	0.377	0.380	0.003
17		5 Fractions	0.368	0.368	0.368	0.000	
18		7 Fractions	0.353	0.344	0.349	0.005	
19		30% ^b	0.317	0.314	0.316	0.002	
20	Bimodal distributions	50% ^b	0.314	0.310	0.312	0.002	
21		70% ^b	0.330	0.324	0.327	0.003	

589

Table 3. Simulated porosity with varied rebounding probabilities (a, standard deviation)

ID	Rebounding Probability	Addition Rate			Extra Timesteps	Windup Timesteps	Simulated porosity				
		Amount	Every Timesteps	Normal Timesteps			1 [#]	2 [#]	3 [#]	Mean	
1	0.1	1	10	7500	0	500	0.437	0.440	0.441	0.439	0
2	0.2	1	10	7500	0	500	0.433	0.436	0.436	0.435	0
3	0.3	1	10	7500	0	500	0.434	0.429	0.432	0.432	0
4	0.4	1	10	7500	0	500	0.434	0.429	0.430	0.431	0
5	0.5	1	10	7500	0	500	0.434	0.438	0.434	0.435	0
6	0.6	1	10	7500	0	500	0.433	0.433	0.438	0.435	0
7	0.7	1	10	7500	0	500	0.446	0.447	0.443	0.445	0

590

Table 4. Simulated porosity with varied addition rates (a, standard deviation)

ID	Rebounding Probability	Addition Rate			Extra Timesteps	Windup Timesteps	Simulated porosity				
		Amount	Every Timesteps	Normal Timesteps			1 [#]	2 [#]	3 [#]	Mean	
1	0.25	1	2	1500	0	500	0.460	0.463	0.457	0.460	0
2	0.25	1	5	3750	0	500	0.446	0.448	0.441	0.445	0
3	0.25	1	10	7500	0	500	0.434	0.432	0.434	0.433	0
4	0.25	1	20	15000	0	500	0.424	0.427	0.428	0.427	0
5	0.25	1	30	22500	0	500	0.423	0.421	0.422	0.422	0
6	0.25	1	40	30000	0	500	0.421	0.421	0.420	0.421	0
7	0.25	1	50	37500	0	500	0.420	0.420	0.421	0.420	0

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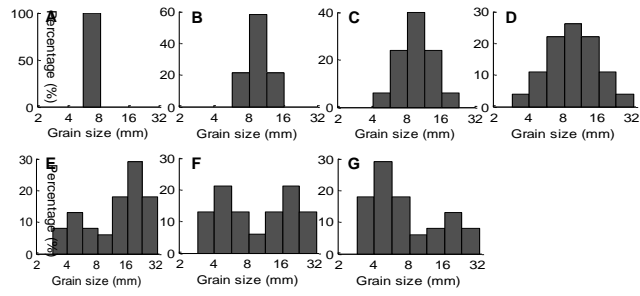
Table 5. Simulated porosity with varied windup timesteps (a, standard deviation)

ID	Rebounding Probability	Addition Rate			Extra Timesteps	Windup Timesteps	Simulated porosity				
		Amount	Every Timesteps	Normal Timesteps			1 [#]	2 [#]	3 [#]	Mean	
1	0.25	1	10	7500	500	0	0.434	0.435	0.437	0.435	0
2	0.25	1	10	7500	500	1000	0.432	0.432	0.434	0.433	0
3	0.25	1	10	7500	500	2000	0.434	0.431	0.433	0.433	0
4	0.25	1	10	7500	500	4000	0.435	0.432	0.435	0.434	0
5	0.25	1	10	7500	500	8000	0.432	0.434	0.432	0.432	0
6	0.25	1	10	7500	500	16000	0.434	0.433	0.436	0.435	0
7	0.25	1	10	7500	500	32000	0.431	0.432	0.430	0.431	0

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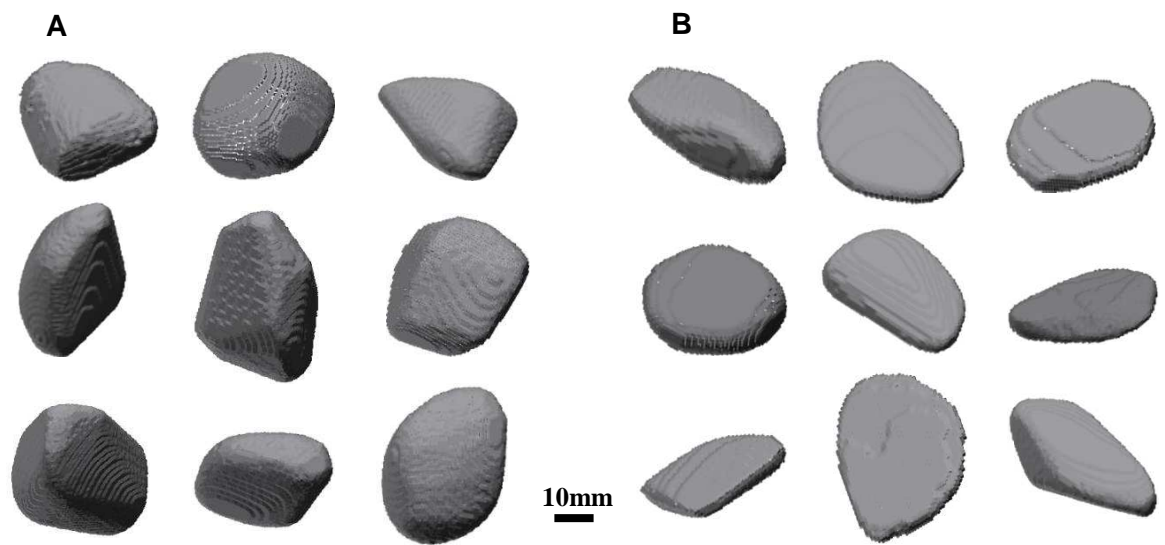


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596 **Fig.1**

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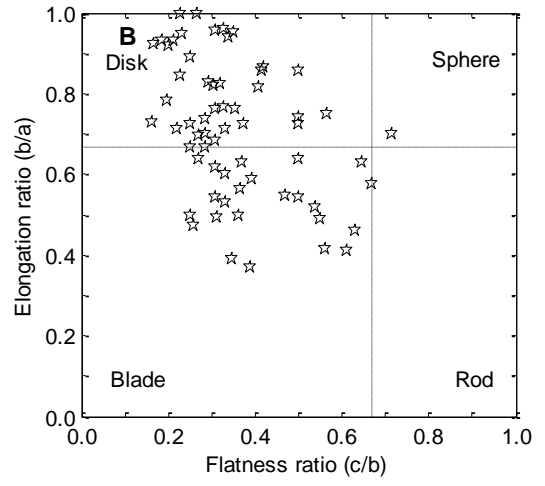
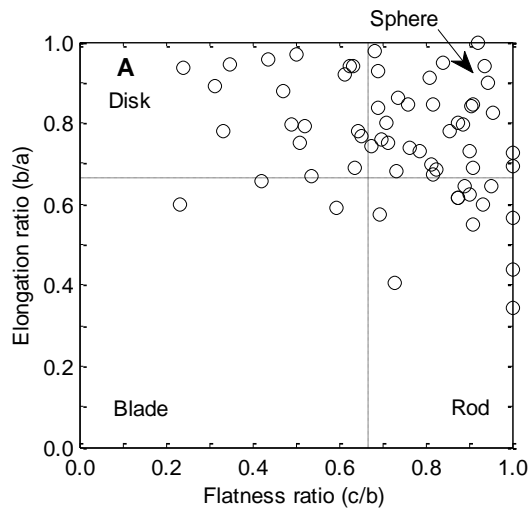
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601 **Fig.2**

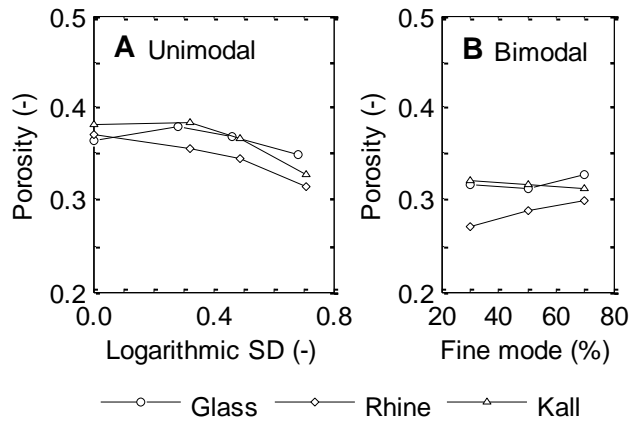
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604 **Fig.3**

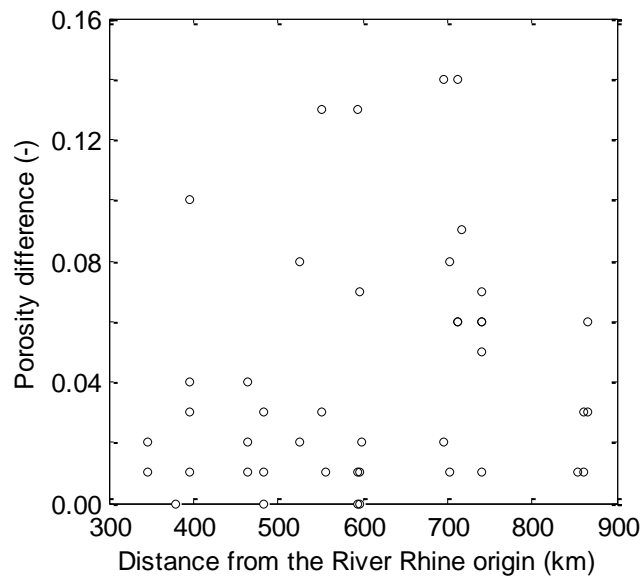
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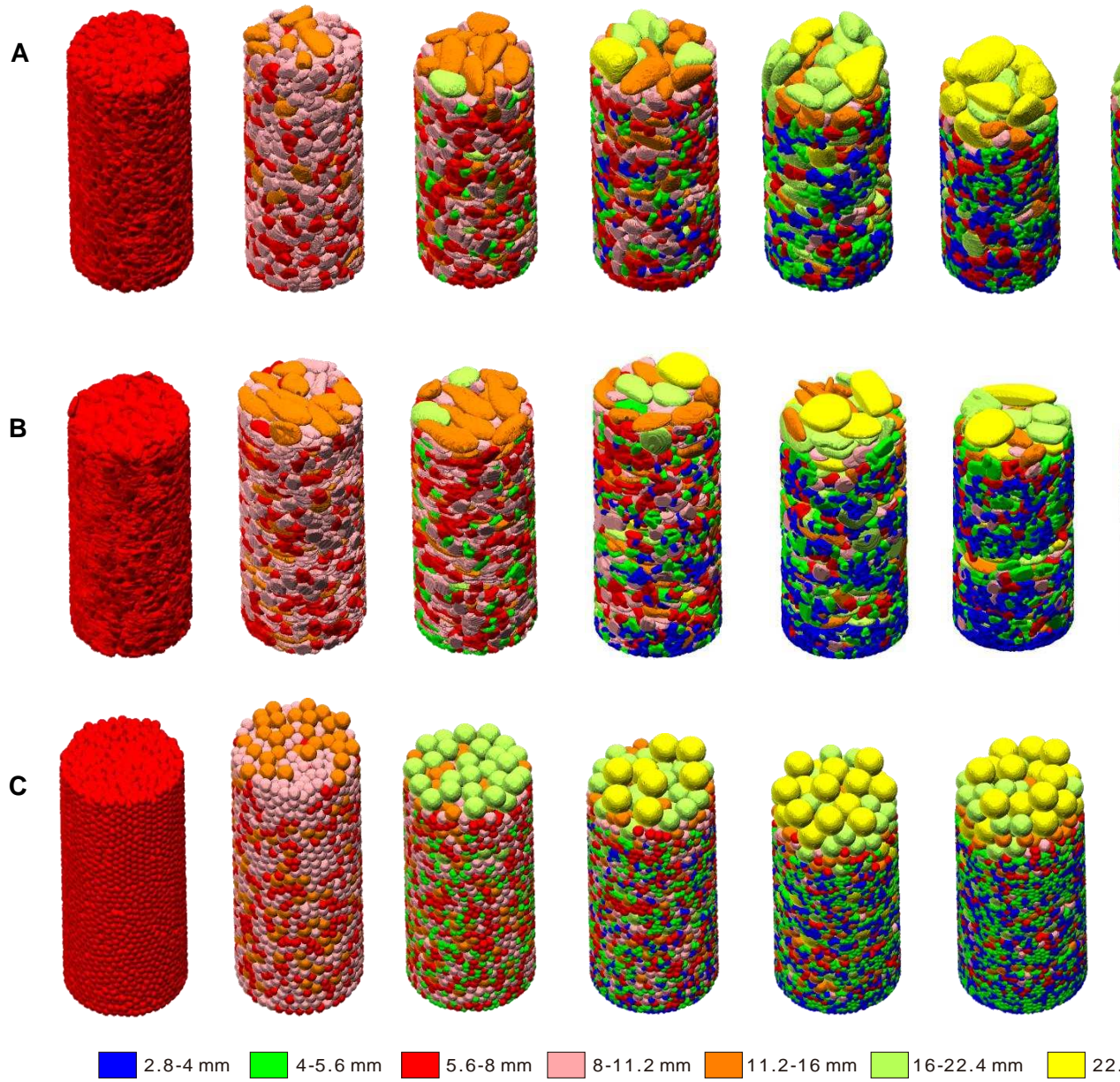
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607 **Fig.4**

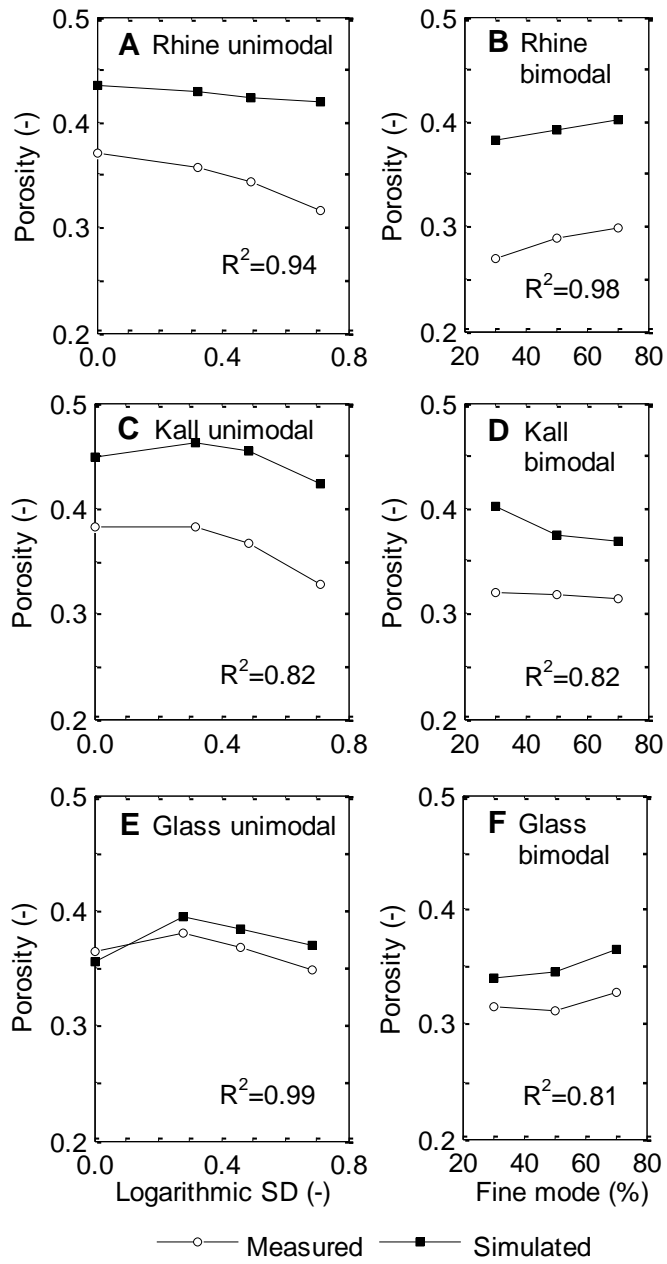
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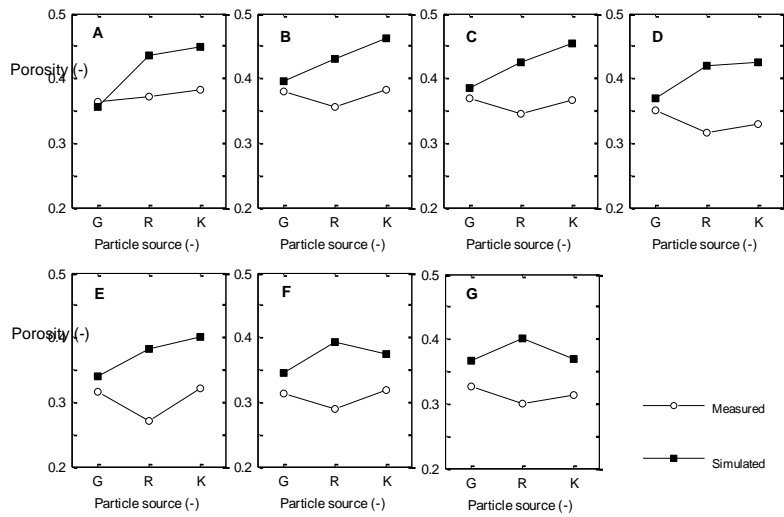
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 610 **Fig.5**
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 613 **Fig.6**
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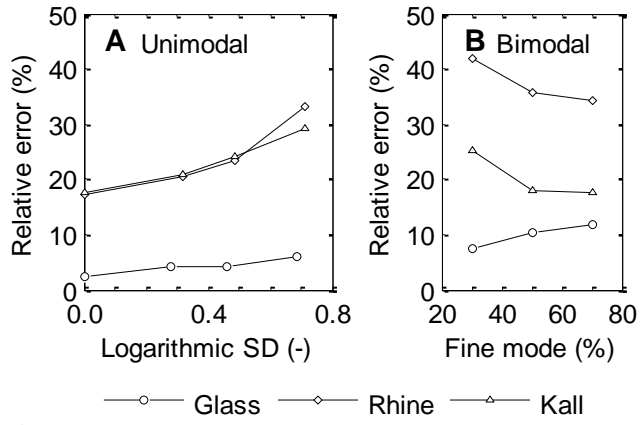


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617 **Fig.7**



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620 **Fig.8**

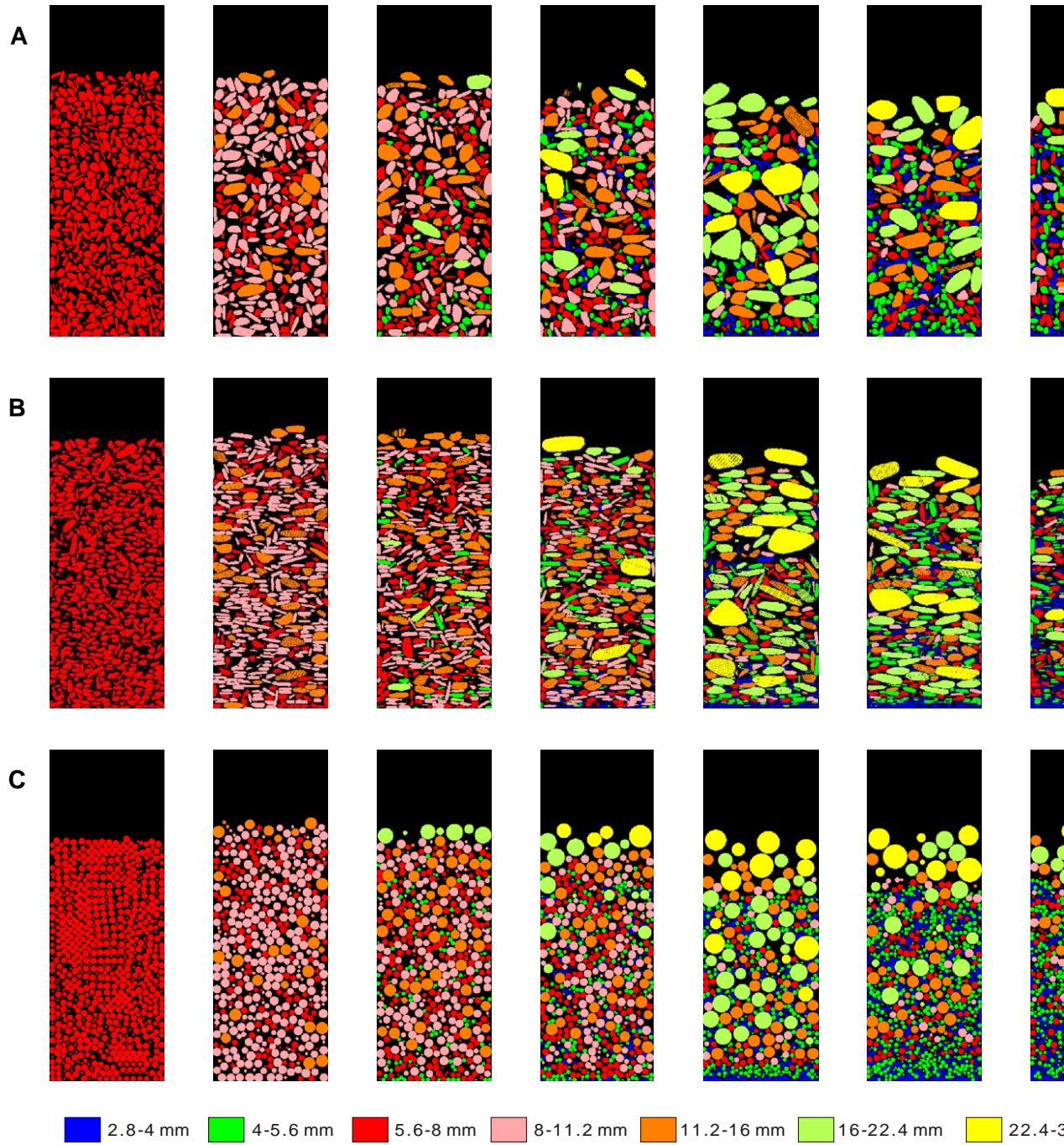
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Fig.9

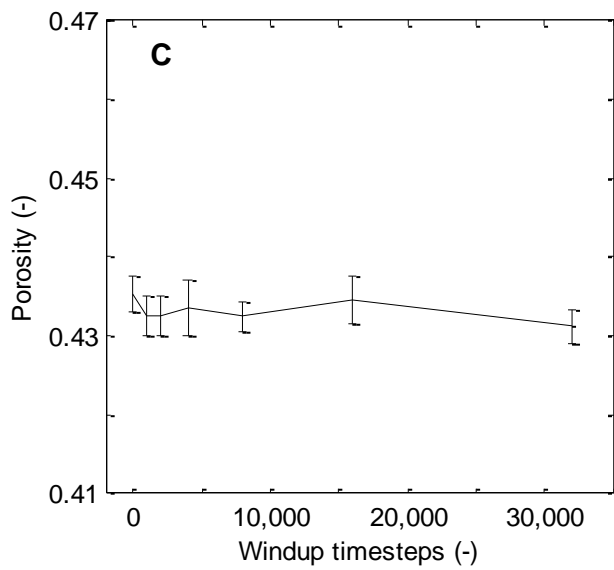
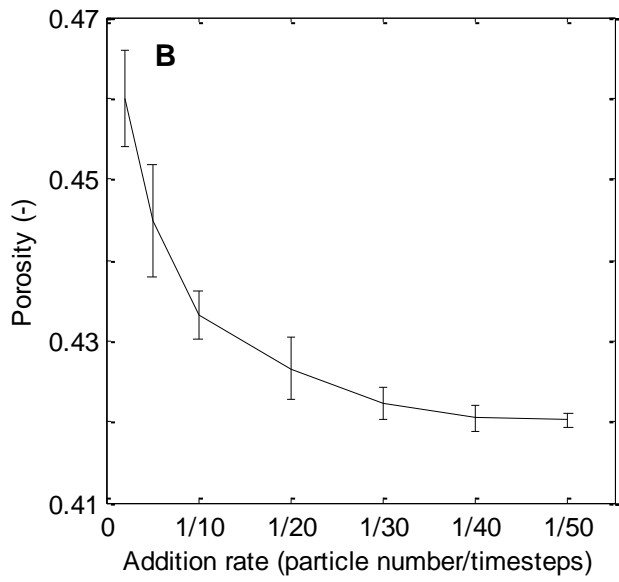
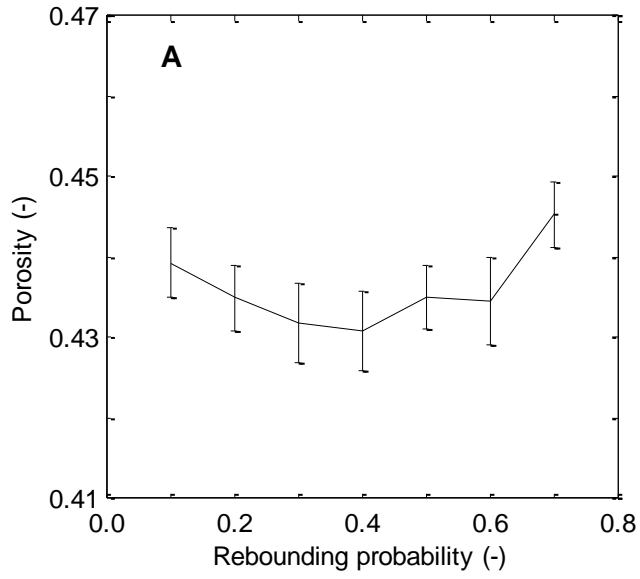
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Fig.10

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629 **Fig.11**

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