

Coarse-Grained Geological Porous Media Structure Modeling Using Heuristic Algorithm and Evaluation of Porosity, Hydraulic Conductivity, and Pressure Drop with Experimental Results

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1 **Coarse-Grained Geological Porous Media Structure Modeling Using**
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9
10 **Abstract**

11 Knowledge of porous media structure is an essential part of the hydrodynamic investigation of
12 fluid flow in porous media. To study soil behavior (as a granular porous media) and water and
13 contaminant movement in the vadose zone, appropriate estimation of soil water retention curve
14 (SWRC) and soil hydraulic conductivity curve (SHCC) has a pivotal role and is one of the most
15 challenging topics for researchers and engineers in soil and water science. The SWCR can be
16 approximated using an accurate particle size distribution (PSD) function. In this study by
17 applying random close packing (RCP) method as an encouraging method for predicting and
18 studying particle configuration, an optimal particle size distribution is developed for coarse-
19 grained soils ($0.025 \text{ mm} < \text{PSD} < 3.35 \text{ mm}$). The mentioned RCP is generated using heuristic
20 algorithm with merging applicable equations of soil science. For porous media modeling,
21 MATLAB software is used and the predicted results by the optimal model for the parameters
22 of porosity, pressure drop, and saturated hydraulic conductivity are compared with laboratory

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23 measurements. Experimental design is conducted by MINITAB and predicted coarse-grained
24 soils structure by the model is compared with 4 sifted soils. The results of the sensitivity
25 analysis showed that the porosity obtained from the model is strongly sensitive to the resolution
26 factor and should be chosen with a sufficiently large amount (higher than 250). Results showed
27 good consistency (up to 95%) between predicted porosity and only 10% difference in pressure
28 drop and permeability with observed measurements.

29 **Keywords:** SWRC, Porous Media, Random Close Packing, Heuristic Algorithm, Pressure
30 Drop, ASTM D2434-68

31 **1 Introduction**

32 Soil water retention curve (SWRC) is a powerful and instructive tool to prognosticate soil
33 behavior and water and contaminants movement in the vadose zone. (Tong et al. 2012). SWRC
34 describes the soil matric suction (h) as a function of volumetric soil moisture (θ) or vice versa
35 and along with soil hydraulic conductivity curve (SHCC) is utilized to estimate soil hydraulic
36 properties (Braddock et al. 2001). There are several empirical and theoretical methods for
37 predicting SWRC in literature. The ASTM D6836-16 has been developed to laboratory
38 measure SWRC consisting five standard methods (A to E) at various suction ranges (Leong
39 2019). Another conventional laboratory method for estimating SWRC is to use the particle size
40 distribution (PSD) curve and volume-mass properties (Wen et al. 2020). One of the theoretical
41 methods is to apply the pore size distribution function (PoSD) and develop soil characteristic
42 curve based on the soil pores network (Chen et al. 2019; Fredlund et al. 1994). It should be
43 noted that unlike PSD, PoSD is affected by climatic conditions (temperature, soil moisture
44 content, number of rainy or rainless months) and even could change with soil shrinkage (Wen
45 et al. 2021). Of course, some physical-based conceptual models have been propounded to
46 predict SWRC. In these models, by using an appropriate PSD function and then conversion to

47 PoSD, SWRC is modeled ([Arya and Paris 1981](#); [Assouline and Rouault 1997](#); [Zhai et al. 2020](#)).

48 In most of cases, particles and pores are assumed as solid spheres and void cylinders,
49 respectively. However, the fundamental weakness raised about conceptual models is that they
50 do not consider spheres in the aggregate or packed form in a specified volume. The present
51 study focuses on this important gap, so that by eliminating it an optimal function for PSD are
52 provided. In recent years porous media structure prediction by computer modeling has become
53 one of the researcher's favorite topics. Random close packing and pore network modeling
54 (PNM) methods are used in many types of research and engineering sciences such as studying
55 composite structures ([Wu et al. 2010](#)), distribution and loading of catalyst beds in chemical
56 reactors ([Dorai et al. 2012](#)), study of different polymers ([Ch et al. 2013](#)), hydrocarbon-bearing
57 reservoir rock ([Al-Dhahli et al. 2013](#)), microstructure and powder-based structures material
58 ([Benabbou et al. 2010](#); [Zhou et al. 2009](#)), packing cartons problems ([Wu et al. 2017](#)), etc. In
59 mathematics, the problem of packing particles in a limited space is a subset of optimization
60 problems. In RCP method, solid particles are assumed as spherical, cylindrical, and cubic or
61 pyramid ([Li et al. 2010](#)). Depending on the complexity and structure of considered media, using
62 a combination of these figures is suggested. RCP method investigates the packing and relation
63 of solid particles in scale under consideration. On the other hand, porosity, void spaces and
64 channels' connections are subject of PNM method. In this method (for instance in 2D state),
65 the channels and throats between particles are considered as circles and rectangles, respectively
66 ([Xiong et al. 2016](#)). Euler approach is the prominently used approach in RCP and Lagrange
67 approach is so in PNM method. Therefore, the results are not so different from each other.
68 Particles could be used in the same size or with a size distribution ([Baranau and Tallarek 2014](#);
69 [Daneyko et al. 2011](#); [Santiso and Müller 2002](#)). Packed media with spherical particles then
70 compared on their porosity and coordination number. Particle density defined as total solid
71 volume to total volume ratio and coordination number is the number of particles in the vicinity

72 of a specific particle (Anikeenko et al. 2008; Farr and Groot 2009). Porosity can be calculated
73 from particle density. In RCP method, mechanical contraction, Monte Carlo, particle drop and
74 roll, spherical growth, and Lubachevsky–Stillinger (L–S) algorithm are among important
75 rudimentary algorithms (basic algorithms) for the construction of porous media (Hitti and
76 Bernacki 2013; Kansal et al. 2002; Kyrylyuk et al. 2009; Tobochnik and Chapin 1988). Hybrid
77 or heuristic methods commonly are a combination of the above algorithms or algorithms with
78 improved and coupled equations. For the mechanical contraction (sedimentation) algorithm
79 introduced by Williams and Phillips (2003), first, all particles are generated in a finite space
80 using a random distribution function. In order to minimize the space occupied by the particles
81 and achieve the desired porosity, the particles' z-coordinate is reduced as much as possible
82 based on their initial position. According to the definition of the non-overlap constraint for
83 solid particles, each particle is sedimented vertically until it reaches the bed of stable stationary
84 particles. The most important drawback of this method is the creation of unconventional spaces.
85 This algorithm is strongly dependent on the initial position of the generated particles in the
86 studied volume. Although by changing the diameter of the particles and their initial position,
87 this problem can be partially eliminated, but in any case, achieving the optimal arrangement is
88 one of the main problems of this method. In the spherical growth algorithm, after producing
89 the first particle as the central nucleus (core) of the set, considering the minimum particles
90 distance and non-overlapping conditions, the first layer of particles is created in the vicinity of
91 the desired particle. In this method, the growth of the layers surrounding the central core is
92 circular (for 2D assumption). By increasing the circumfluent boundary of particles, the
93 computation time increases significantly. Because the newly loaded particle sweeps the entire
94 boundary of the set to achieve the optimal position (minimum distance from the central core)
95 (Bargmann et al. 2018). He et al. (1999) proposed the Monte Carlo method for producing
96 particles with different sizes in an arbitrary finite volume. According to the Monte Carlo

97 algorithm, all particles are produced in completely initial random coordinates and smaller than
98 their actual size. Then, by concerning the non-overlapping and volume interference constraints,
99 the particles' volume is increased to achieve a dense arrangement with the desired density and
100 porosity. Like the mechanical contraction method, this method is also affected by the initial
101 position of the generated particles. However, in this method, by replication of the results (for
102 example, up to 10,000 replication), the mentioned problem is eliminated and by averaging the
103 results, the best arrangement and porosity is evaluated. For the drop and roll algorithm,
104 developed by Visscher and Bolsterli (1972), unlike the Monte Carlo and the mechanical
105 contraction methods in which all particles are generated simultaneously, the creation and
106 evaluation of the stable position of the particles are investigated one by one. This method is
107 more complex than previous methods and its calculation time is very long, But the results are
108 more precise. It is worth noting that the RCP method is the starting point for research on porous
109 media. Indeed, after modeling and generation the structure of the porous media, various aspects
110 such as the fluid flow, the rate of thermal resistance (or shape alteration), and the
111 compressibility of the porous media are investigated.

112 As mentioned before, the main objective of this study is to propose modified PSD and an
113 upgraded mathematic model to predict coarse-grained soils structure as a typical granular
114 porous media. The heuristic algorithm which is presented for the first time in this study is the
115 combination of "spherical growth" and "dropping and rolling" by implementation of modified
116 functions in the matrix domain.

117 **2 Modeling and System Parameters**

118 In order to predict the soil structure (sifted soil) RCP method is implemented by MATLAB
119 coding. The heuristic algorithm applied in this study is the combination of “spherical growth”
120 and “dropping and rolling” with some modified equations. Soil particles are assumed as

121 spherical solid particles. In this model objective function is a random distribution of spherical
 122 particles in a finite cubic volume. Whereas soil media is continuum and continuum media
 123 modeling is difficult and more time-consuming, so in the first step, the mentioned cube (called
 124 finite volume) meshed up as depicted in Fig. 1. Discretizing and meshing precision is included
 125 by defining the resolution factor (RF). As shown in Fig. 1, just a set of specified nodes are
 126 utilized instead of the whole points of continuum media. These nodes represent their
 127 surrounding media. Obviously, more node leads to more precision which takes more run time
 128 and RAM capacity. Node numbers depend on the smallest particle size because correct packing
 129 and occupation of each node by particles (spheres) must be guaranteed. Two functions to satisfy
 130 these conditions are defined as Eq. (1) and Eq. (2).

$$RF = f(t_{cal}, d_i, n_i, L_c) \quad (1)$$

$$\varepsilon = g(RF, d_i, n_i) \quad (2)$$

131 In the above equations, t_{cal} points to calculation time, d_i refers to particles (spheres) diameter,
 132 n_i is the number of each particle, L_c is cube edge size, and ε is the estimated porosity. In Fig.
 133 1, grid spacing (called mesh-grid) is obtained by Eq. 3 as follows:

$$L_m = \frac{L_c}{RF} \quad (3)$$

134 In which L_m notes two nodes distance and L_c is cube edge size. Nodes coordination (x_i, y_i, z_i)
 135 is assumed as a center of spheres. It should be noted that in matrix space if the center of enough
 136 large sphere is allocated to an arbitrary grid (sphere whose radius is bigger than two neighbor
 137 node distance), necessarily some of neighboring grids would be enclosed too. Therefore,
 138 necessarily each node is not at the center of a sphere. But surely every sphere is placed at the
 139 center in a randomly selected node (Fig. 2-a). The next step is to define of a random function
 140 for the completely random placing of particles. In each computational step, a group of nodes
 141 occupied by each sphere with an optional radius which produced by the rand function in

142 MATLAB. Normal distribution function, Weibull, and Lognormal are among important
143 random functions in 3-dimensional spaces. Many studies show the best approximation could
144 be obtained using Weibull distribution for size distribution of soils (Esmaelnejad et al. 2016;
145 Rhodes 2008). Therefore, Weibull and normal distribution functions are employed in
146 MATLAB to construct spheres with random diameters. Neglecting these nodes for the next
147 placement is obligatory since counterpart soil particles couldn't overlap each other (Fig. 2-b).
148 It's also an important point to reduce computational time. As it's shown in Fig. 2-b, in 2D space
149 and for a general (i, j) node chosen as circle center point, neighboring nodes also placed inside
150 of the circle so won't be considered again. This important condition is implemented by defining
151 matrixes with zero and one arrays. The matrixes that include number one array represent nodes
152 that have not yet been occupied by the particle. For the next ball (with specified random radius)
153 placement, the nearest node with minimum z to the last sphere would be selected according to
154 Fig. 2-a and Fig. 2-c. Indeed, to increase the computational speed, the probability function is
155 defined for the remaining nodes. In order to place the next sphere, the distance of all remaining
156 nodes from the center of the previous sphere is calculated in the matrix domain. A node which
157 is selected for the center of the next sphere must fulfill two constraints. The minimum distance
158 from the center of the previous sphere and its minimum z_i coordinate. The probability matrix
159 is calculated for all remaining nodes and the node with the largest array (maximum probability)
160 is selected. Obviously, in this case, there will be nodes with equal probability density (Fig. 2-
161 b). After assigning the node as the center of the sphere (with a random radius), the non-
162 overlapping condition is tested by calculating the Euclidean distance of the node from the node
163 allocated to the central core. If the above condition would not true, the node is stored in a matrix
164 called NAN and removed from the calculation cycle, and the next node is chosen with the
165 maximum probability. This cycle is continued until the particle loaded correctly and the next
166 sphere loading calculations is resumed. As mentioned before, the present algorithm is a

167 combination of "spherical growth" and "drop and rolling" algorithms by implementation in
168 matrix space. To apply this idea, the cubic volume which contains particles is divided into m
169 sublayers. Then by using conditional statements to constrain model to necessarily fill the first
170 layer with spheres and do not proceed to the next layer until the previous layer (or nodes)
171 completely filled. After placement of each sphere, this sphere acts as a central (core) sphere for
172 the next adjacent spheres. The 2-dimensional case of this process is represented in [Fig. 2-d](#).
173 Sphere number represents its placing order. Flowchart of all calculations and particles
174 placement in confined volume is shown in [Table 1](#).

175 Our main research goal is to investigate contaminant dispersion in soil. In the first step, we
176 need to have a good estimate of SWRC and SHCC. As mentioned before, one way to predict
177 SWRC is to use the accurate PSD function. In the present study by applying heuristic algorithm
178 the structure and particle configuration of coarse-grained soils are investigated. Besides,
179 properties such as porosity (or saturated volumetric humidity), saturated hydraulic conductivity
180 and pressure drop are evaluated. These parameters are strongly influenced by soil texture and
181 structure. Soil texture indicates the percentage of sand, silt, and clay particles and is an
182 important criterion of soil PSD. However, the structure of the soil explains the configuration
183 and arrangement of these particles. Therefore, we want to know this method of RCP to generate
184 porous media which uses spheres, how closely resembles real media.

185 **3 Material and Equipment**

186 For preparing laboratory coarse-grained soils, a specified amount of soil is collected and sorted
187 by different grain sizes using standard laboratory sieves which are used for gradation test as it's
188 shown in [Table 2](#).

189 In order to ensure uniform PSD for each mesh, screening with a mechanical shaker is repeated
190 three times. A plastic hammer was used during meshing to eliminate dust. Four sets with

191 specific mesh sizes are shown in Fig. 3. Four types of coarse-grained soils are provided by
192 mixing all of the above four particle size groups with mass weight mixing ratios as shown in
193 Table 3. These mixing ratios are also used for modeling coarse-grained soils in MATLAB. For
194 each size classification, Weibull and normal distribution functions are employed. Indeed, to
195 generate spheres with random diameter, four Weibull and normal distribution functions are
196 applied.

197 For a random variable X (diameter of spheres) that takes positive and continuous values, the
198 Weibull probability density function is presented by Eq. (4) as follows:

$$f(x; \lambda, k) = \begin{cases} \frac{k}{\lambda} \left(\frac{x}{\lambda}\right)^{k-1} e^{-(x/\lambda)^k} & x \geq 0 \\ 0 & x < 0 \end{cases} \quad (4)$$

199

200 Where k and λ refer to shape and scale parameters, respectively.

201 3.1 Porosity Measurement

202 In order to porosity measurement of the mentioned laboratory coarse-grained soils, standard
203 stainless steel cylinders (100.00 ml) were filled with them and saturated with water. Cylinders'
204 weight was measured precisely before and after filling with soil and then water. Then the
205 samples were placed in an oven at 105°C for 24 hours to ensure that all its moisture content
206 evaporated. Samples' weight was measured again and porosity was calculated by its difference
207 to previous measurements. For each soil, this experiment was repeated 3 times to ensure the
208 accuracy of the results. The cylinders containing sifted soils are shown in Fig. 4.

209 3.2 Pressure Drop and Permeability

210 One important parameter that affects fluid flow in porous media, is pressure drop due to porous
211 media resistance to flow through pores. Pressure drop increases by effective porosity reduction.

212 A modified equation based on Kozeny-Carmen equation (Rhodes 2008) is utilized to
 213 investigate the pressure drop in the model. For a porous media with identical spherical grain,
 214 pressure drop could be expressed as Eq. (5):

$$\frac{\Delta P}{L} = \frac{180 \mu (1 - \varepsilon)^2}{\varphi_s^2 D_p^2 \varepsilon^3} v_s \quad (5)$$

215 In which ΔP is pressure drop, L is length, μ is dynamic viscosity, v_s is superficial velocity, ε is
 216 porosity, φ_s is sphericity (which is equal one for a perfect sphere) and D_p is equivalent grain
 217 diameter. Using Darcy law and rearranging Kozeny-Carman equation, the permeability of a
 218 porous media with identical sphere grain could be written as below:

$$v_s = \frac{k \Delta P}{\mu L} \quad (6)$$

$$k = \frac{\varphi_s^2 D_p^2 \varepsilon^3}{180 (1 - \varepsilon)^2} \quad (7)$$

219 Permeability and saturated hydraulic conductivity relation could be expressed by Eq. (8):

$$k = K_s \frac{\mu}{\rho g} \quad (8)$$

220 In which k is the permeability of porous media in m^2 , K_s is hydraulic conductivity in $m.s^{-1}$, μ
 221 is dynamic viscosity in $kg.m^{-1}.s^{-1}$, ρ is fluid density in $kg.m^{-3}$ and g is gravity acceleration in
 222 $m.s^{-2}$ (Loll et al. 1999). To precisely estimate the saturated hydraulic conductivity of groups of
 223 jammed sphere grains with different diameters, Irani and Callis (Irani, C.F., Callis 1963)
 224 equation is used (Eq. 9a-9d). This applicable equation represents the equivalent mean diameter
 225 for a group of soil particles with different sizes.

$$\sigma_g = e^b \quad (9-a)$$

$$d_g = e^a \quad (9-b)$$

$$a = 0.01 \sum_{i=1}^n f_i \text{Ln } M_i \quad (9-c)$$

$$b = 0.01 \sum_{i=1}^n f_i \text{Ln}^2 M_i - a^2 \quad (9-d)$$

226 In which d_g is the mean diameter of grains, σ_g is the variance of grain size distribution, n is the
 227 number of different grain size groups, and f_i is the mass percent of grains which has diameter
 228 equal or less than M_i in each group. Following the recommendation for application of geometric
 229 mean diameter to sieved sediments, M_i is taken as the arithmetic mean of two consecutive
 230 particle size limits (Shirazi and Boersma 1984). Therefore, by using the mentioned equation
 231 and also using Weibull and normal distribution functions to generate spheres with different
 232 diameters, the mean diameter is calculated for four types of sifted soils.

233 3.3 Laboratory investigation of pressure drop

234 ASTM D 2434-68 is used for measuring pressure drop and saturated hydraulic conductivity in
 235 soil porous media. This standard is used to measure the pressure drop and hydraulic
 236 conductivity of disturbed granular soils in saturated conditions. Setup of the experiment is
 237 shown in Fig. 5. Sifted soils from previous steps (65 kg), are used for experiments.

238 3.4 Experimental Design Method

239 By applying "Minitab" software and general full factorial design method, the order of
 240 experiments is completely randomized. Each experiment is repeated three times to assure the
 241 validity and accuracy of the results. Total number of 72 experiments are carried out. 6 treatment
 242 of 49, 59, 69, 79, 89, and 95 cm water head (constant water head) are used for four soil types.
 243 Due to using sifted soil particle which has specific grading, it is expected that pressure drop
 244 would be the same for the equal depth of column as soil prepared homogenously.

245 4 Modeling and Laboratory Results

246 The model result for type 1 soil structure is delineated as an example in Fig. 6. Also, the
247 structure of the coarse-grained soil for the particle size distribution of 25 microns to 3350
248 microns is shown in Fig. 7. Comparison of the results between normal and Weibull distribution
249 functions showed that the Weibull distribution function has much better results in estimating
250 soil porosity. In the next step, to reduce the difference between the estimated and empirical
251 porosity, the skewness and elongation coefficients of the Weibull distribution function (in the
252 terms of shape and scale parameters) were inclined to negative values. As a result, the use of
253 the modified Weibull distribution function led to the development of an optimal RCP model
254 for predicting porosity. According to the symmetric shape of the normal distribution function
255 (around the mean value of each desired grain size range), its skewness coefficient is zero and
256 its default elongation coefficient is 3. Comparison of the siefted soils porosity and the
257 corresponding optimal RCP model showed that the average relative error between the two
258 porosities is less than 4%. While for the normal distribution function, the predicted porosity
259 showed larger values and the relative error percentage was up to 8.9%. The predicted values of
260 porosity by mathematic optimal model and experimental data for four types of soils is presented
261 in Fig. 8. The most important parameters in determining the porosity of the porous medium
262 were replication, resolution factor, and particle size distribution function. Modeling of particles
263 configuration carried out in two modes which were the least and most effective magnitude.
264 While the rest of the parameters were assumed to be constant (see Table 4). The results of the
265 sensitivity analysis showed that the porosity obtained from the model is strongly sensitive to
266 resolution factor and should be chosen with sufficiently large amounts. The results are
267 represented in Fig. 9. By using a modified distribution function for sphere diameter and
268 choosing a high-Resolution factor ($RF > 250$), the relative error of porosity reduced to less than
269 3%. By normal distribution function and $50 < RF < 100$, relative error up to 10% obtained.

270 Resolution factor is a criterion of discretization accuracy and the number of nodes in the cube.
271 For example, for a cube with a length of 1cm and RF=200, there would be 8×10^6 nodes. In this
272 case, it's obvious that run time increases exponentially too (over 10 hours for RF=200 and a
273 week for RF=300). By approaching higher RF values and using the appropriate conditional
274 clause in Weibull distribution function, we could obtain spheres which closely approximate the
275 real condition and build an optimum model with a more precise answer, but it needs higher
276 computational power and run time. The predicted results for pressure drop reveals that Weibull
277 distribution function gets a more accurate result than normal distribution function (Fig. 10). As
278 porosity value obtained by models overestimates real values, accordingly calculated pressure
279 drops are less than measured values. This could be the result of Irani and Callis equation error
280 in estimating mean diameter and Boersma's (Shirazi and Boersma 1984) proposed relation to
281 calculate the arithmetic mean particle diameters for each grain classification. The average
282 difference between actual pressure drop and estimated by the RCP model (using the normal
283 distribution function) was 23.3%. While by applying the modified Weibull distribution
284 function, this difference was reduced to less than 10%. As is expected, almost in all experiments
285 such result for $\Delta P/L$ was observed in manometers which is shown in Fig. 11. Saturated
286 hydraulic conductivity of sifted soils (in the range of sandy soils) was measured using ASTM
287 D 2432-68 and it was compared with model estimates. As an example, Estimated saturated
288 hydraulic conductivity and measured values for soils type one and two are shown in Fig. 12.
289 As previously explained, the modified Weibull distribution function is used to reduce the
290 pressure drop difference to less than 10%. Subsequently, given Eqs. (5) and (7), saturated
291 hydraulic conductivity values are predicted up to 10% larger than the actual values.

292 **5 Conclusion**

293 In this research innovative algorithm is employed to generate sandy soil porous media which
294 is the combination of “dropping and rolling” and “spherical growth” algorithms. The main
295 advantage of this algorithm is the utilization of continuous media discretization method and
296 transforming to matrix space which could successfully model porous media. Also, by using
297 applied equations in soil science, and modified Weibull distribution function, an optimal RCP
298 model was developed to predict the parameters of porosity, pressure drop, and saturated
299 hydraulic conductivity. Comparison of the results of the optimal model and laboratory
300 investigations reveals that the difference between the predicted and measured porosity is less
301 than 4%. A difference of 10% is also observed for the parameters of pressure drop and saturated
302 hydraulic conductivity. One of the unique characteristics of this model is building completely
303 organized and structured porous media which happens for equal and monodispersed spheres in
304 the range of $30 < RF < 70$ (represented in [Fig. 13](#)).

305 **6 Future Study**

306 Providing a suitable model to predict SWRC has always been a favorite of researchers. By
307 applying a proper PSD and also ratios of fine sand/silty clay mixtures to their maximum
308 densities, we can propose a conceptual model to prognosticate SWRC with acceptable
309 accuracy. Indeed, after finding the PSD, using the suggested equations, we will try to obtain
310 the corresponding PoSD function, and finally, SWRC will be predicted based on PoSD.

311

312 **7 Abbreviation**

313 **RCP:** Random Close Packing

- 314 ***PNM***: Pore Network Modeling
- 315 ***SWRC***: Soil Water Retention Curve
- 316 ***SHCC***: Soil Hydraulic Conductivity Curve
- 317 ***PSD***: Particle Size Distribution
- 318 ***PoSD***: Pore Size Distribution
- 319 **Appendix. Nomenclature**

d	diameter (m)	<i>Greek</i>	
D_p	equivalent grain diameter (m)		
f	mass percent	ΔP	pressure drop ($\text{Kg.m}^{-1}.\text{s}^{-2}$)
g	gravity acceleration (m.s^{-2})	ε	porosity
h	matric suction (m)	θ	volumetric water content ($\text{m}^3.\text{m}^{-3}$)
k	permeability of porous media (m^2)	λ	scale parameters
K_s	saturated hydraulic conductivity (m.s^{-1})	μ	dynamic viscosity ($\text{Kg.m}^{-1}.\text{s}^{-1}$)
L	length (m)	ρ	density (Kg.m^{-3})
L_c	cube edge length (m)	σ	variance of grain size distribution
L_m	mesh grid (m)	ϕ_s	sphericity factor
m	number of sublayers		
n	number of particles	<i>Subscripts</i>	
n_i	number of particles in specific diameter range	i, j, k	counter
RF	resolution factor	c	cube
t_{cal}	calculations time	g	grain
v_s	superficial velocity (m.s^{-1})	p	particle
x, y, z	nodes coordination (m,m,m)	s	saturated

320

321

322

323

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429 ***TABLE captions:***

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431 ***Table 2.*** U.S. standard mesh sieve sizes and numbers.

432 ***Table 3.*** Mixing ratio for four sifted soil by their mass weight.

433 ***Table 4.*** Low and high values of the effective parameters for prediction the porosity (soil type

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449 **Figure 7.** (a) Simulated structure of the granular porous media for particle size distribution of
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451 **Figure 8.** Comparison of predicted and measured porosity values.

452 **Figure 9.** Sensitivity analysis results for prediction of porosity (soil type 1).

453 **Figure 10.** Comparison of estimated and measured pressure drop; (a) soil type 1 and (b) soil
454 type 2.

455 **Figure 11.** Equal pressure drop along soil column in monometers.

456 **Figure 12.** Comparison of predicted and measured saturated hydraulic conductivity (soil type
457 1 and 2).

458 **Figure 13.** Structured random close packing generated by presented algorithm.

459

460 Table 1. Algorithm used to generate porous media with arbitrary spheres

Algorithm:	
1	Inputs: the set of radius $\{r_i\}$, the desired density $(1-\varepsilon)$
2	Calculate the cube size l to achieve density $(1-\varepsilon)$
3	Create the grid network $[g_x, g_y, g_z]c$ along three dimension based on resolution parameter RF
4	Place the first sphere in the $p_1=[r_1/2, r_1/2, r_1/2]$
5	Set $z=z_{min}$ and $P_i=\{p_i\}$, $i=2$.
6	Remove the grid points that would be in a first sphere.
7	While $i \leq$ Number of spheres
8	Calculate the average center C_{avg} equal to mean of P_i in each dimension.
9	$r_{next} = r_i$
10	Calculate the Euclidean distance between all grid networks from C_{avg} and keep them in <i>distance_avg</i> .
11	Set the <i>distance_avg</i> of grid points that leads to collision of dedicated spheres to be a large number.
12	Find the minimum value of <i>distance_avg</i> and place the next sphere's center in this grid point p_i .
13	Add the p_i to P_i .
14	Remove the grid points that would be in this sphere.
15	$i=i+1$.
16	End While.
17	Output: the P_i determines the place of all the spheres.

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Table 2. U.S. standard mesh sieve sizes and numbers

Mesh Number *	6	10	16	30	50
Standard mesh size (mm)	3.35	2	1.18	0.6	0.3
<i>* The standard sieve number indicates the number of holes per square inch of sieve</i>					

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Table 3. Mixing ratio for four soils by their mass weight

	*Type 1	Type 2	Type 3	Type 4
0.3-0.6 mm	3	2	1	1
0.6-1.18 mm	3	2	1	1
1.18-2 mm	1	2	2	3
2-3.35 mm	1	1	2	3
<i>* Type points out the assumed mixing ratios. For example, each 6 kg prepared soil type 1 consists of 3, 3, 1, and 1 kg of soil particles in the range of 0.3-0.6 mm, 0.6-1.18 mm, 1.18-2 mm, and 2-3.35 mm, respectively.</i>				

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Table 4. Low and high values of the effective parameters for prediction the porosity (soil type 1)

	low value	high value	most likely	pessimistic porosity (%)	optimistic porosity (%)
Parameters					
Resolution Factor	50	300	150	47.41	43.89
Distribution Function	Normal	Weibull	Weibull	41.33	44.37
Replication	1	10	3	44.92	44.52
Measured Porosity	43.26%				

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The authors declare that they have no known competing financial interests or

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personal relationships that could have appeared to influence the work reported

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in this paper.

Figures

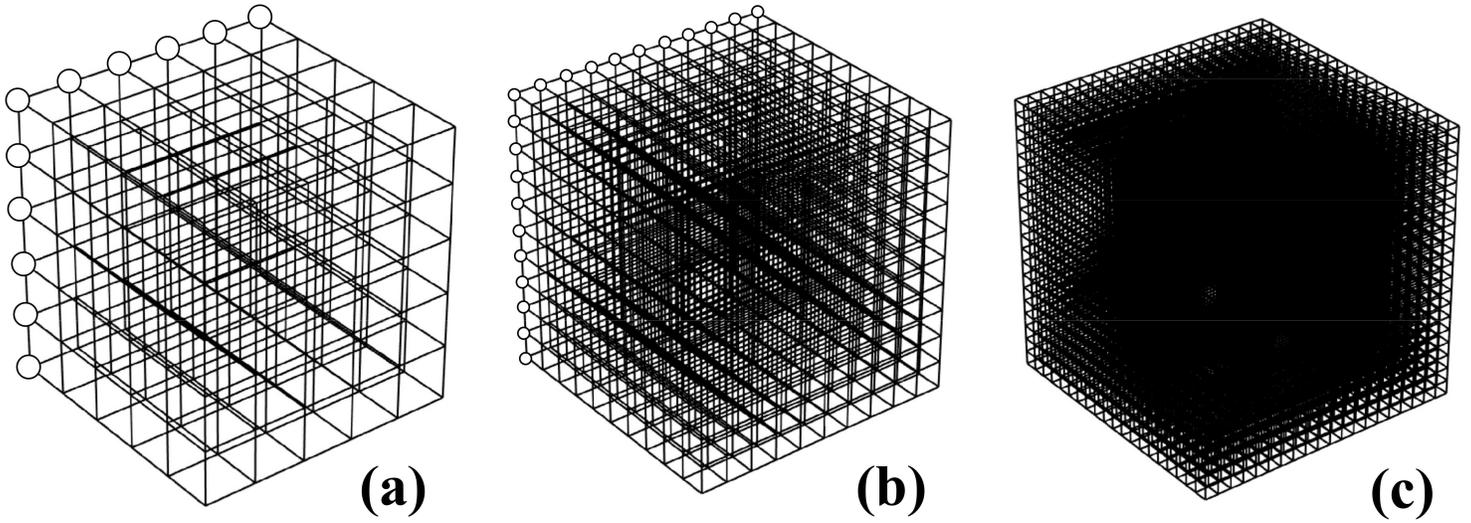


Figure 1

Discretization of continuum space and transformation to solvable matrix space in MATLAB. (a) RF=5, (b) RF=10, (c) RF=20.

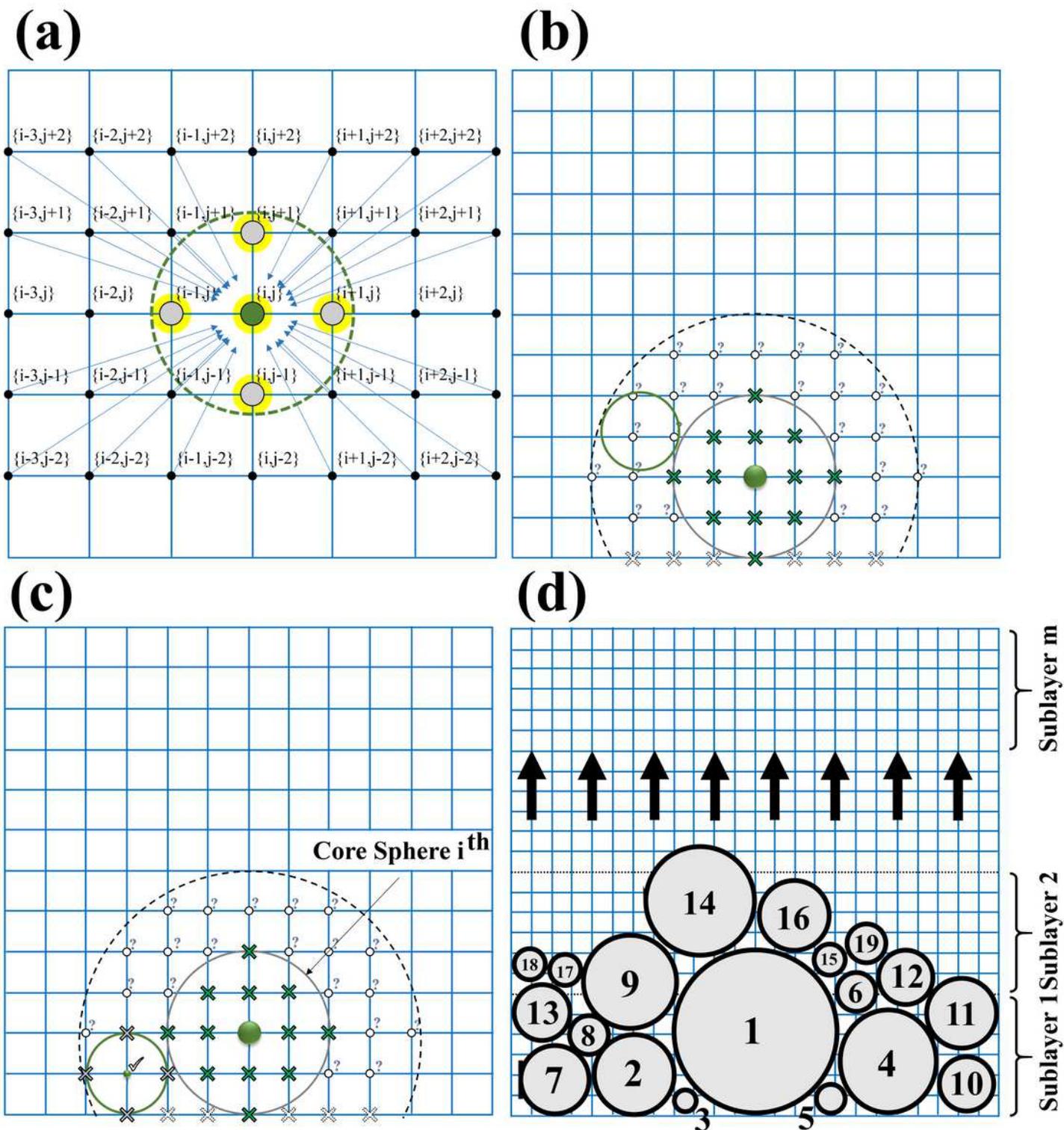


Figure 2

(a) Schematic of spheres allocation procedure and (b), (c) examination of overlap condition and probability matrix using Euclidean distance. (d) Generation and placing of spheres by suggested heuristic algorithm.

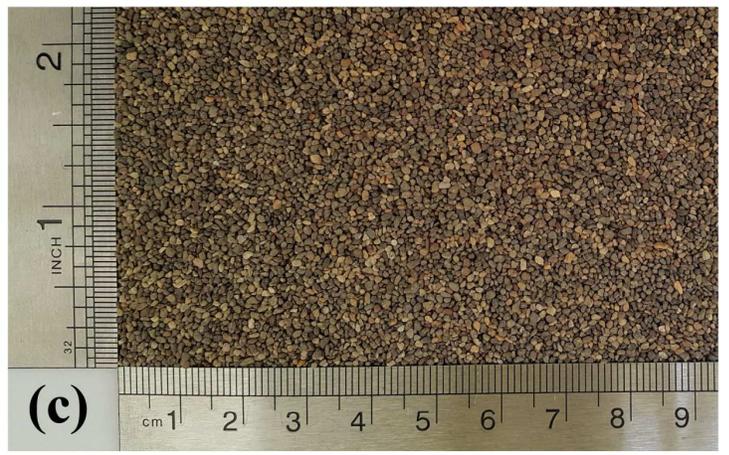


Figure 3

Sifted soil grains with different grading. (a):2-3.35 mm, (b):1.18-2mm, (c):0.6-1.18mm, (d):0.3-0.6mm



Figure 4

Prepared soil samples for porosity measurement.

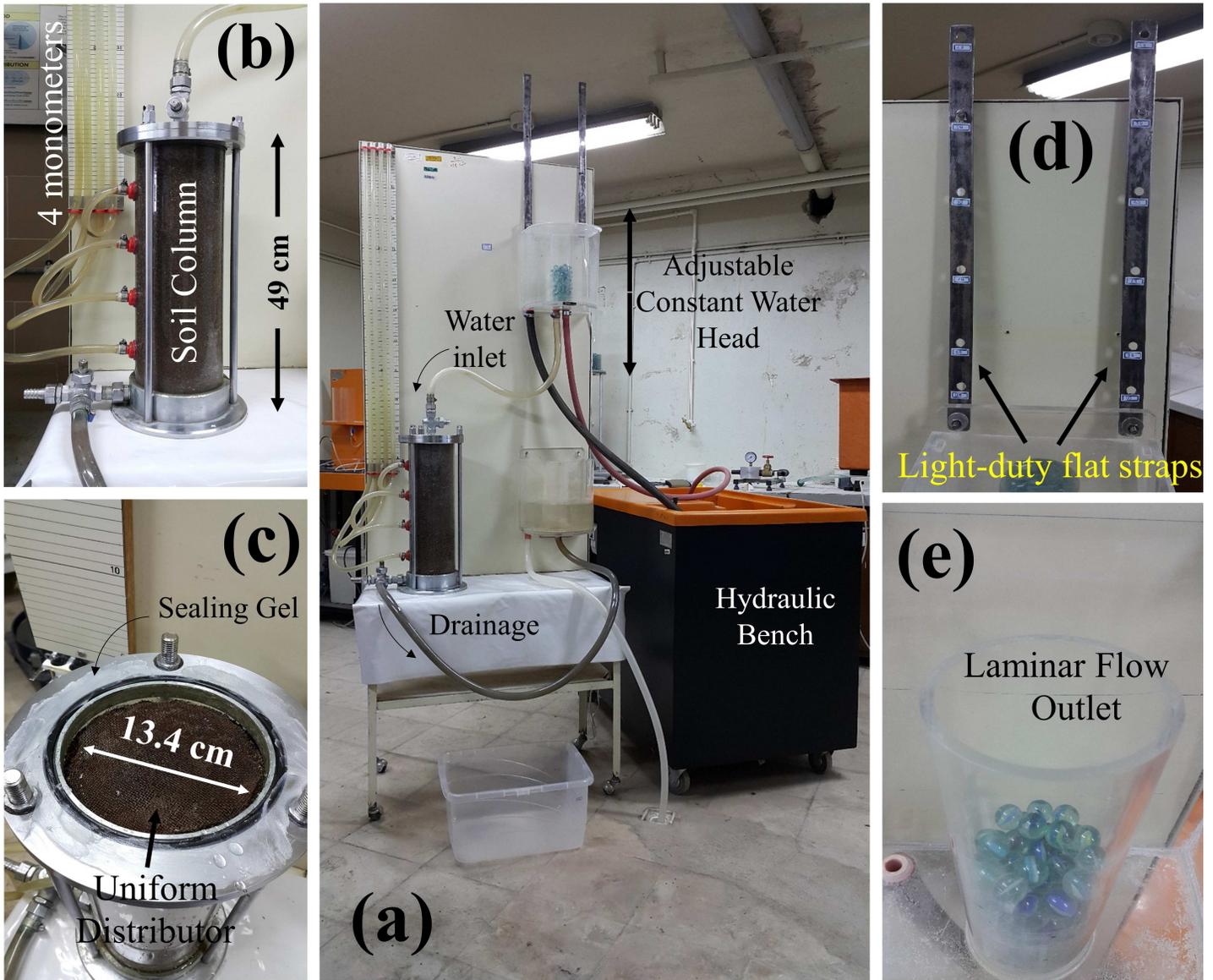


Figure 5

Hydraulic conductivity and pressure drop measurement setup based on ASTM D 2434-68, (a) schematic of the pilot, (b) Soil column with inlet and outlet and 4 manometers, (c) Uniform distributor at column entrance and sealing gel (D) Light-duty flat strap designed to increase or decrease water head, (e) Glass marbles used to prevent flow turbulence

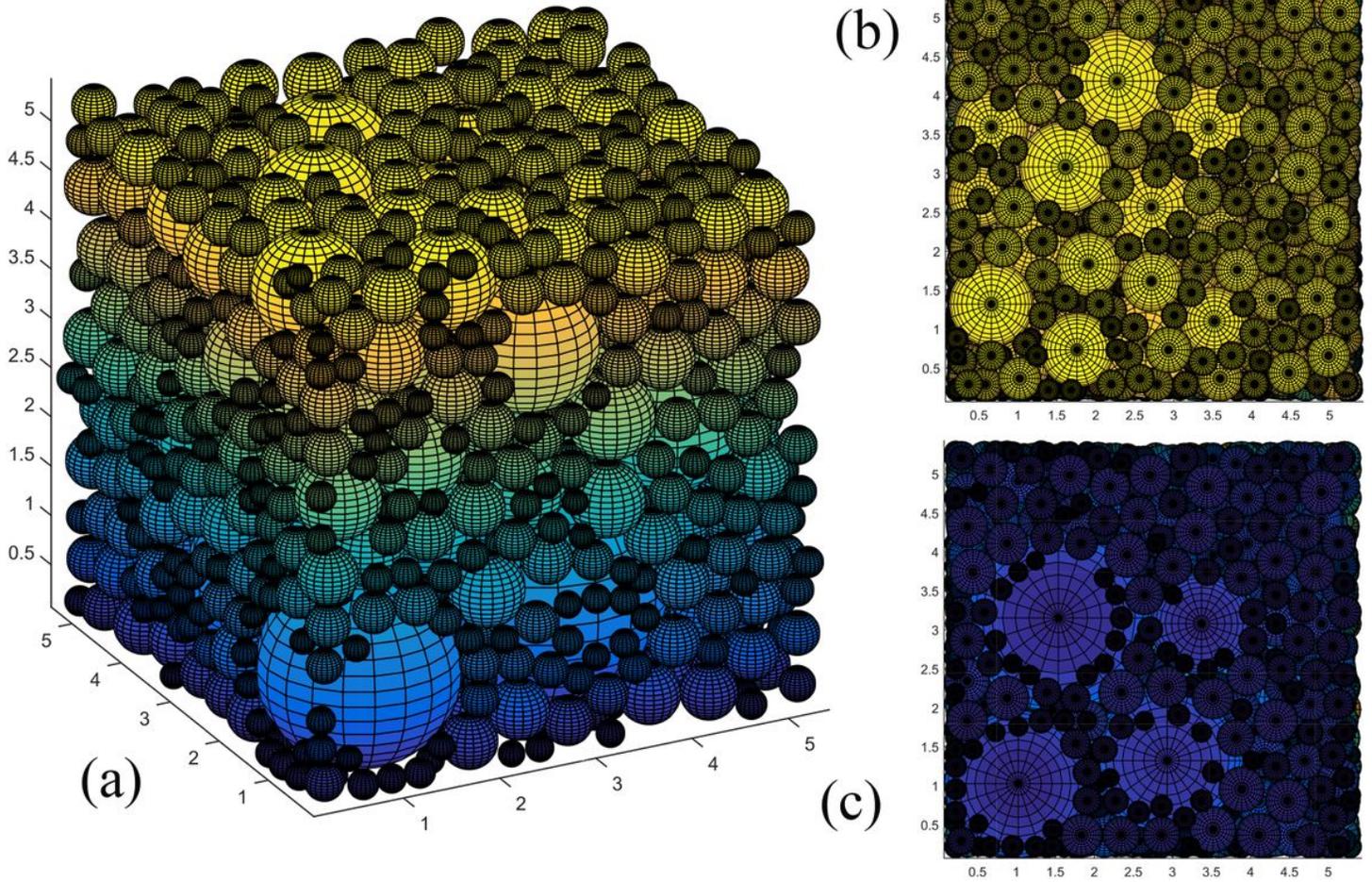


Figure 6

(a) Simulated Porous media structure for soil type one, (b) top and (c) bottom view.

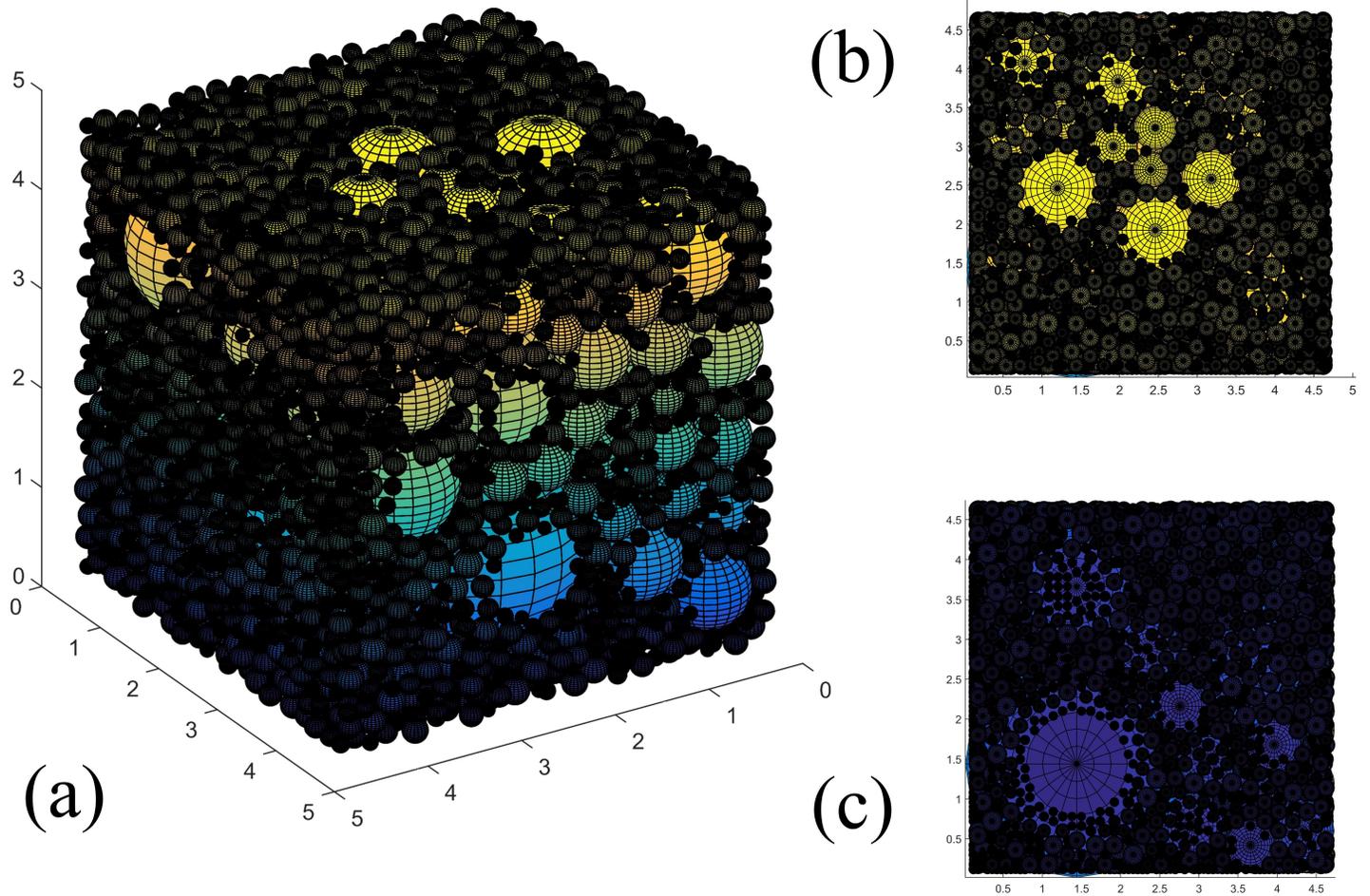


Figure 7

(a) Simulated structure of the granular porous media for particle size distribution of 25 microns to 3350 microns, (b) top and (c) bottom view.

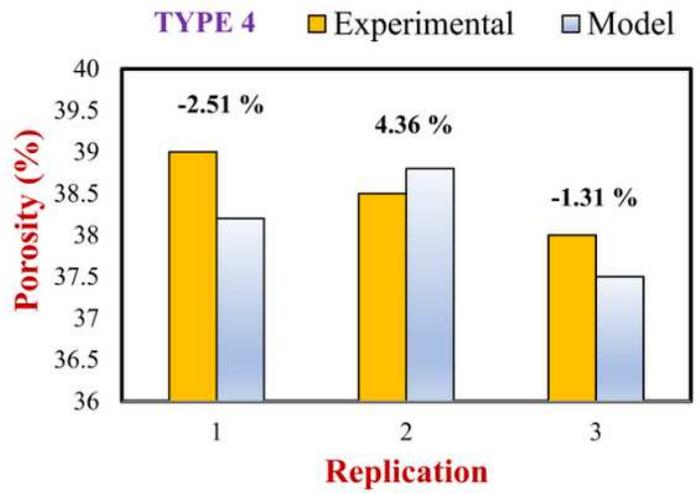
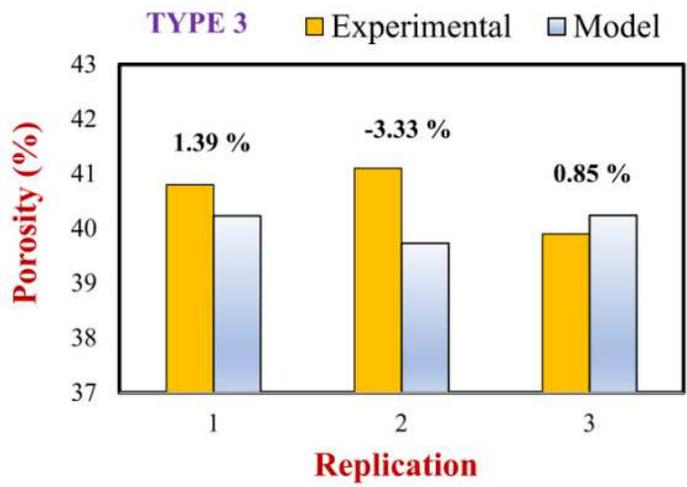
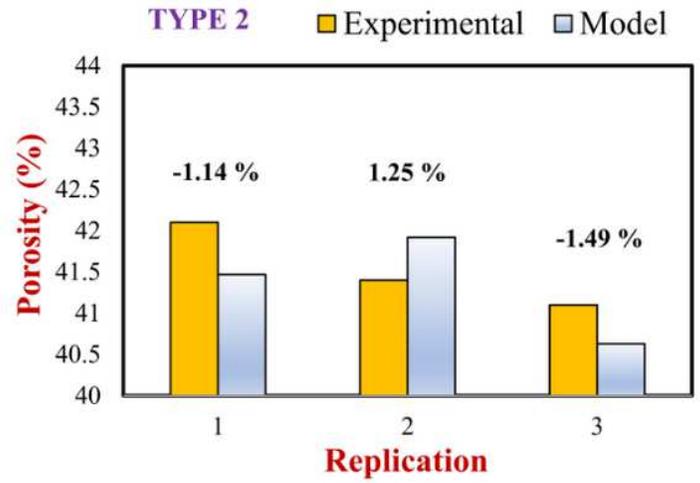
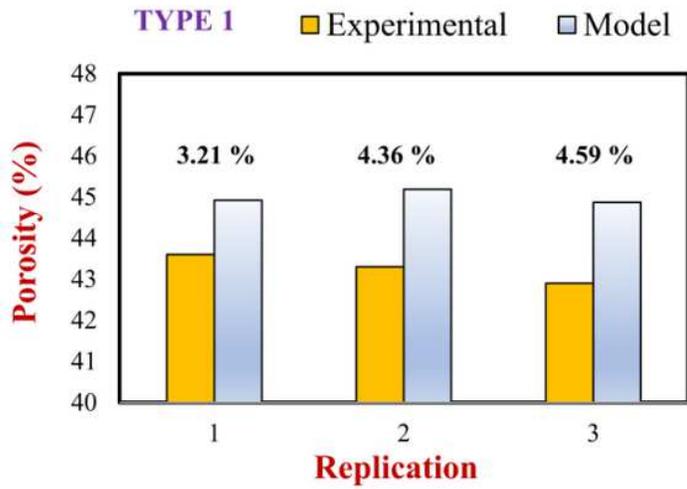


Figure 8

Comparison of predicted and measured porosity values.

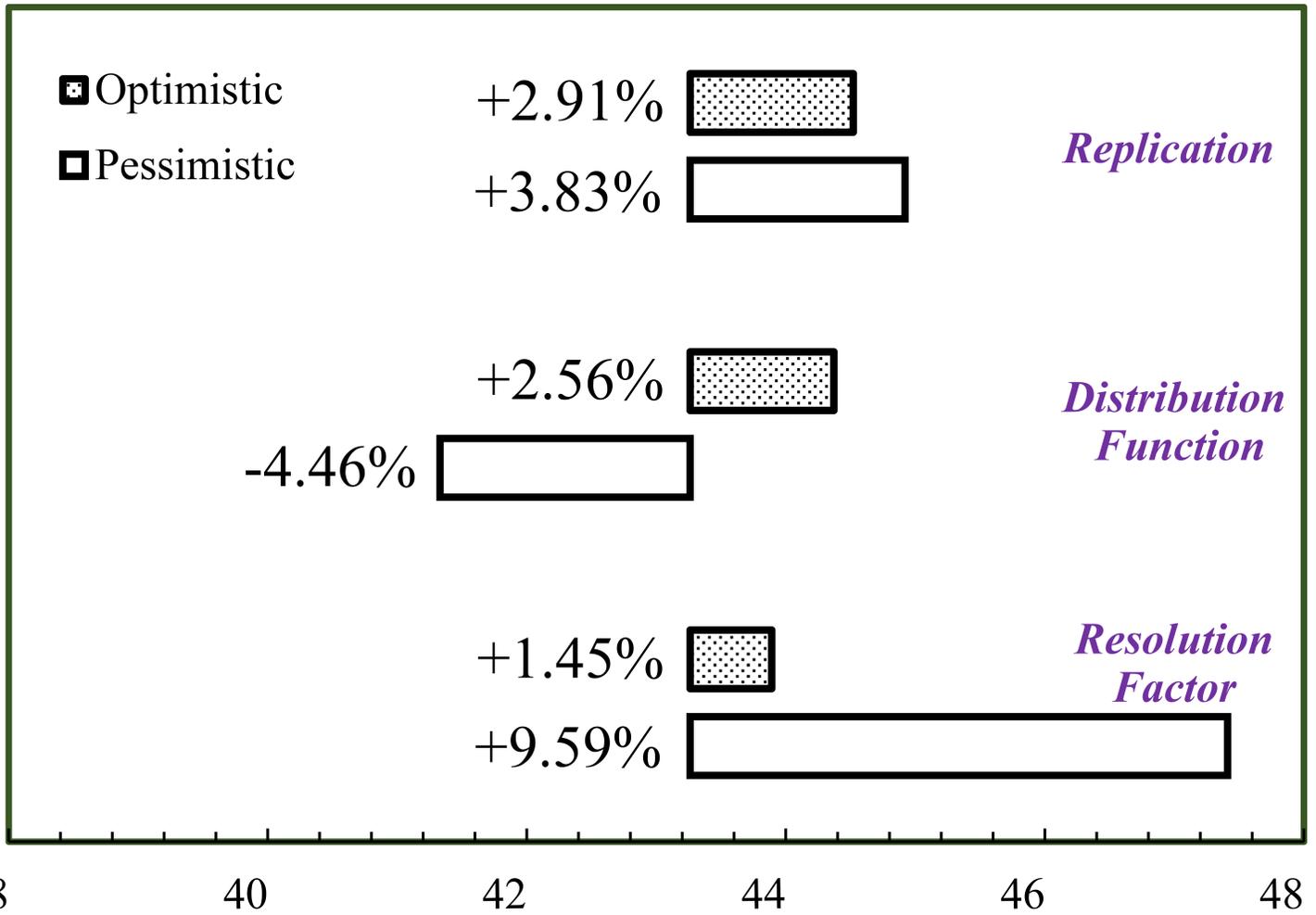


Figure 9

Sensitivity analysis results for prediction of porosity (soil type 1).

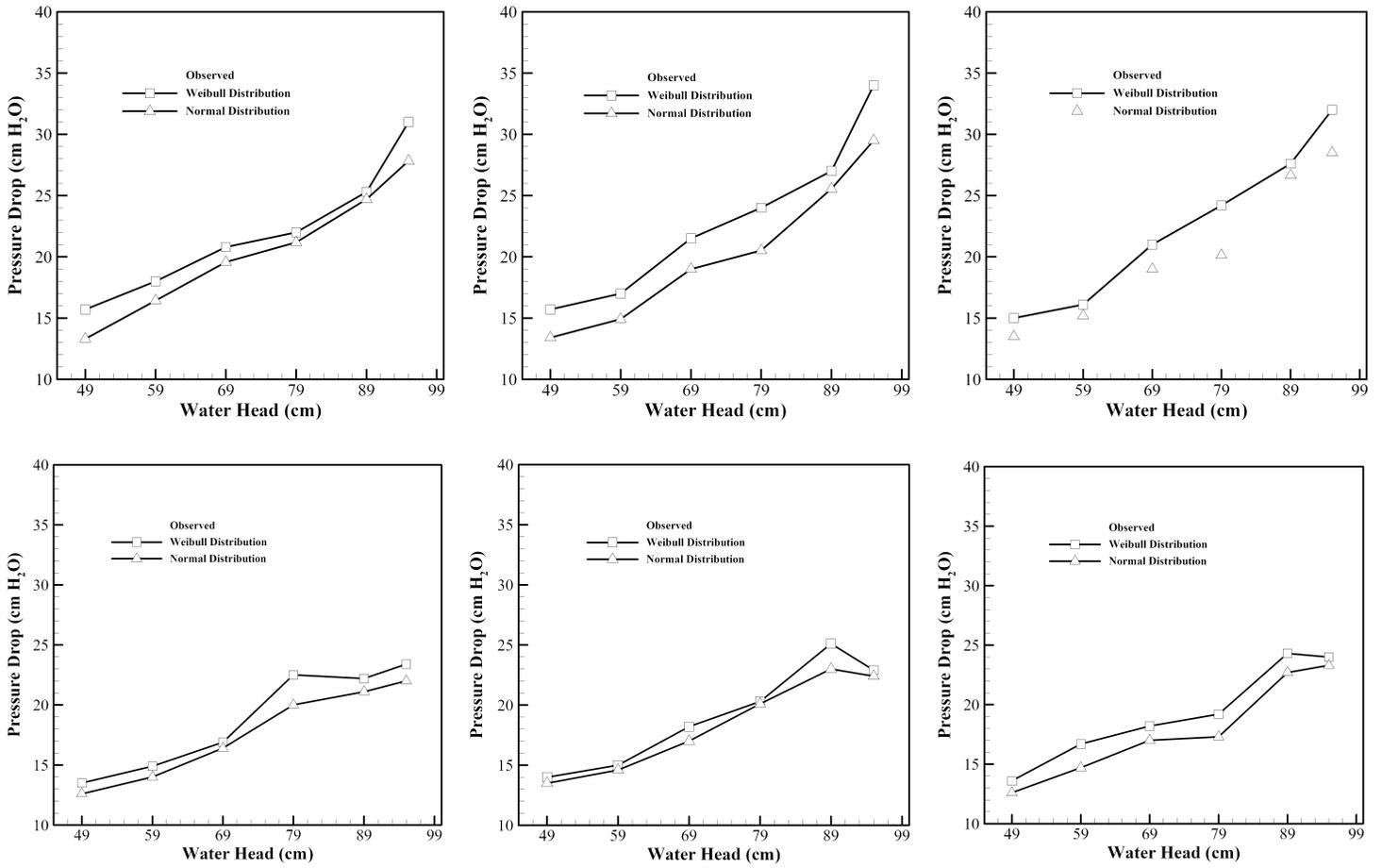


Figure 10

Comparison of estimated and measured pressure drop; (a) soil type 1 and (b) soil type 2.

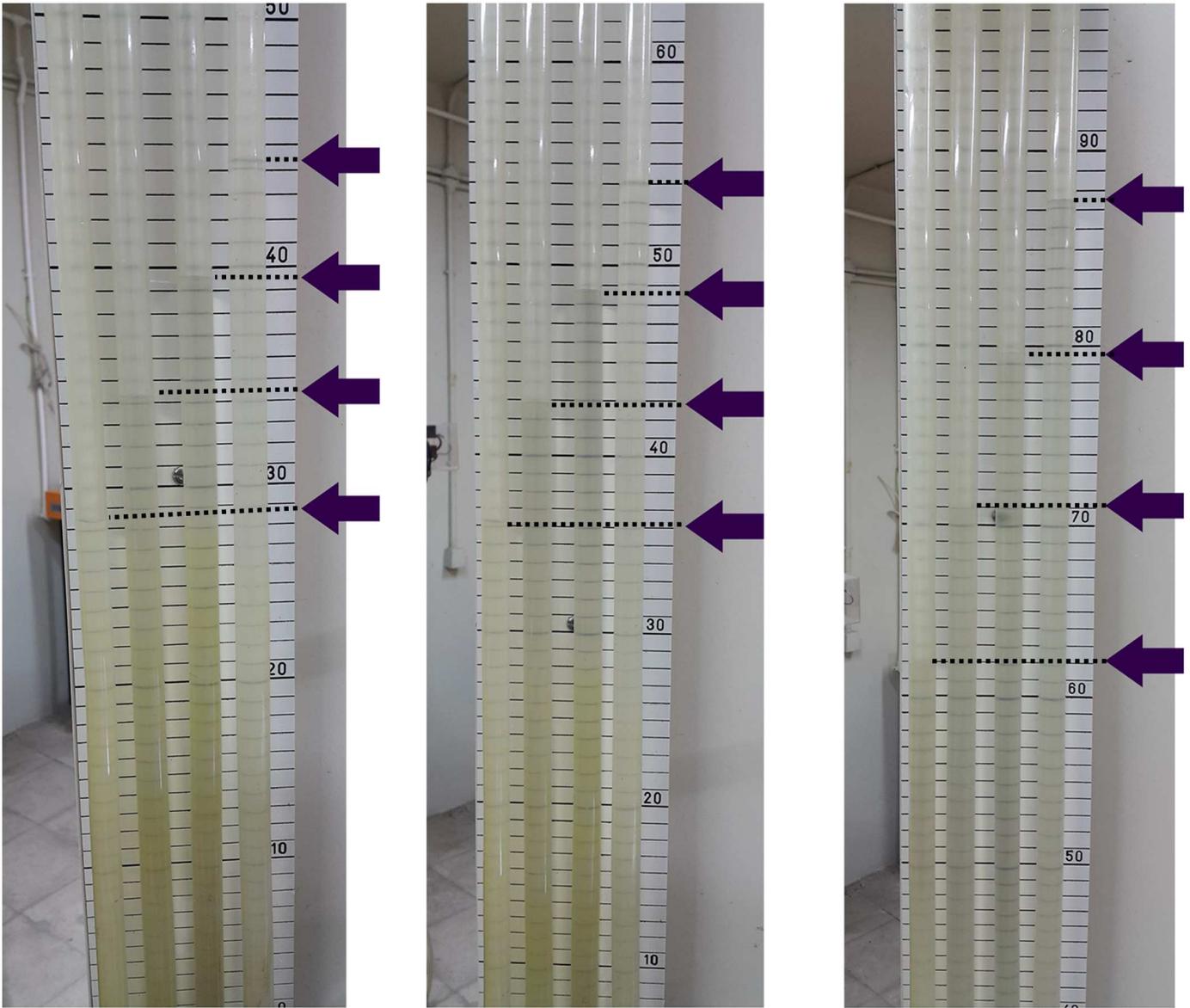


Figure 11

Equal pressure drop along soil column in monometers.

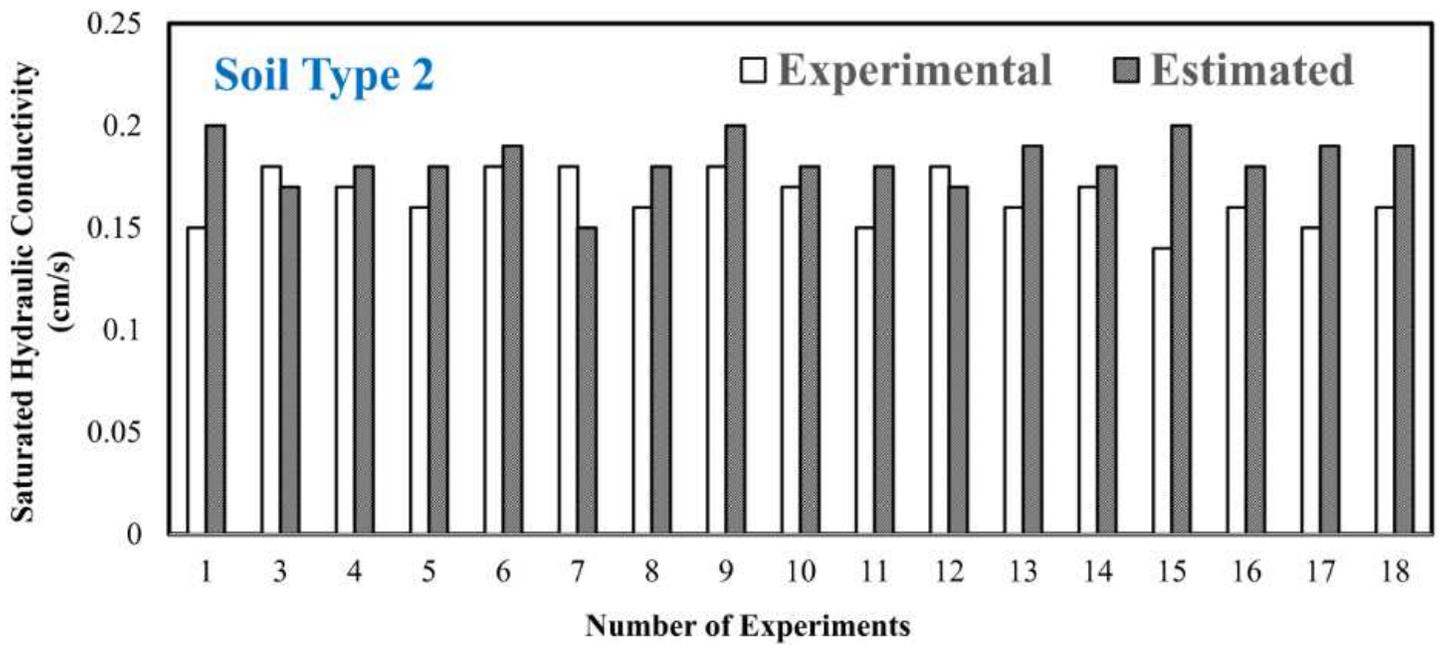
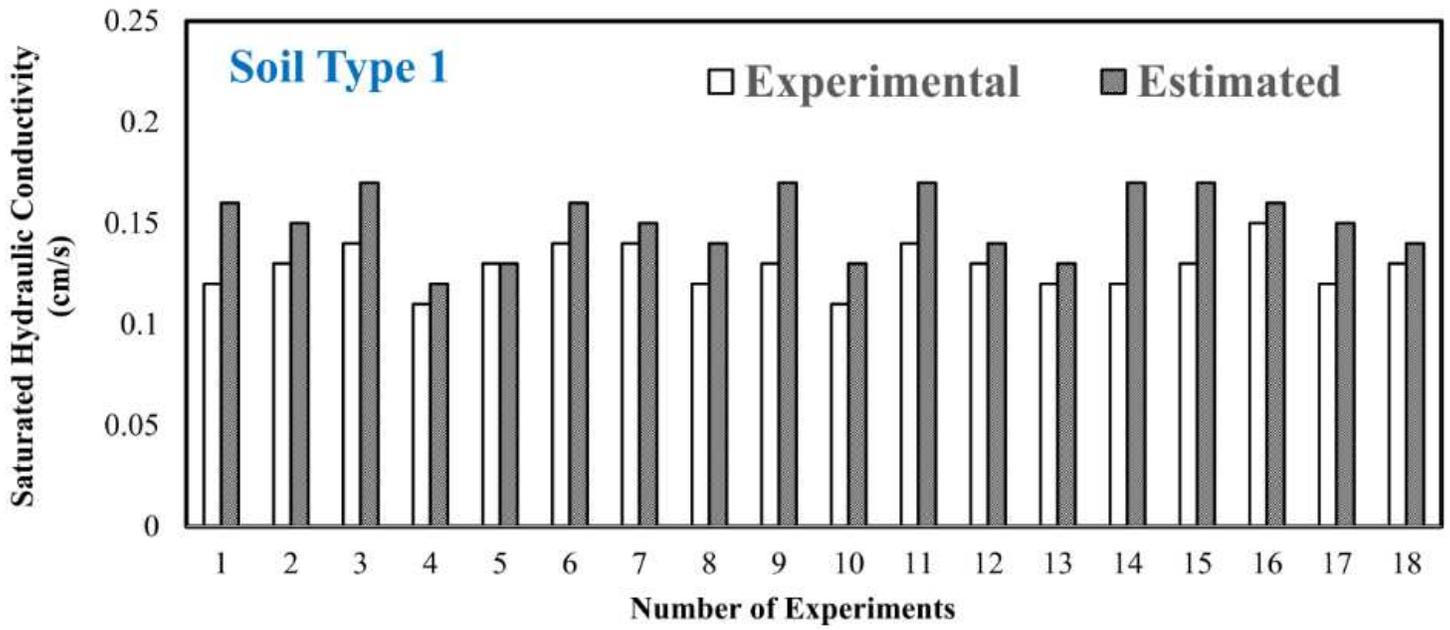


Figure 12

Comparison of predicted and measured saturated hydraulic conductivity (soil type 1 and 2).

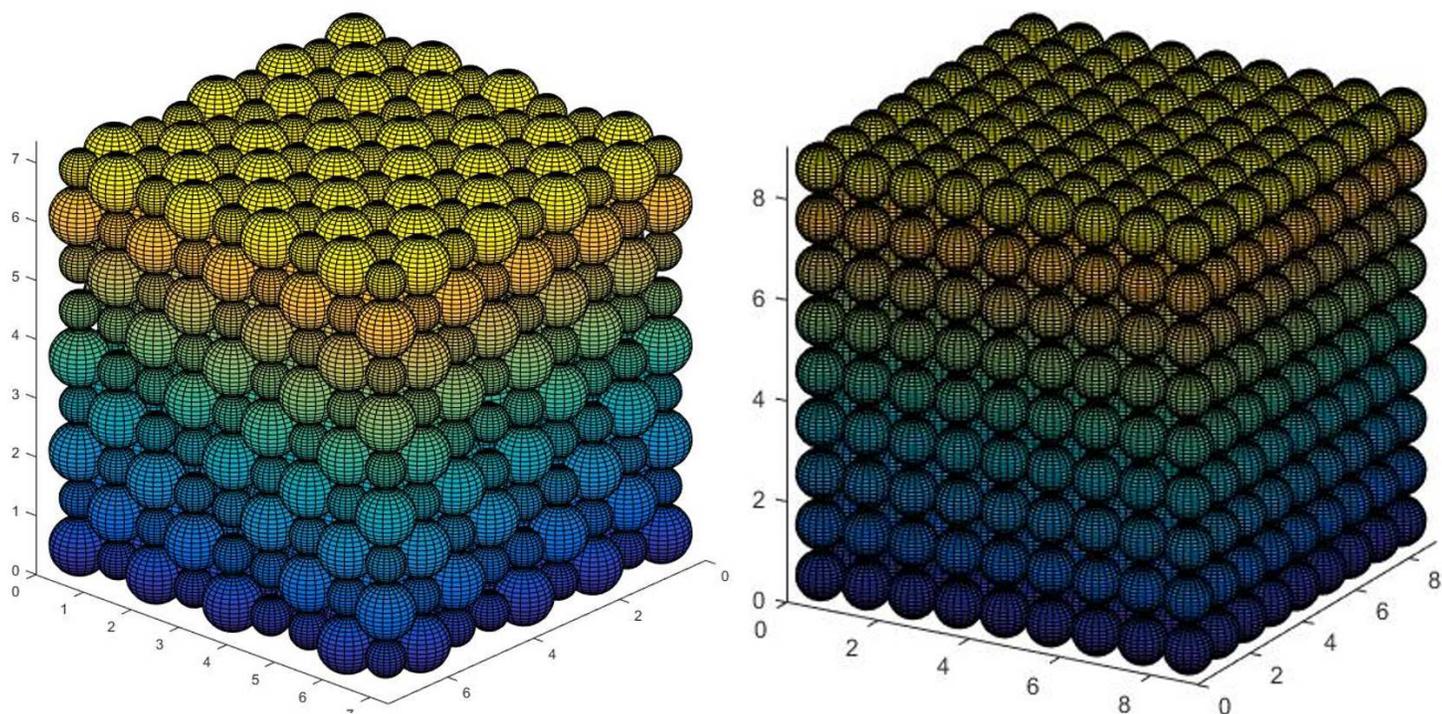


Figure 13

Structured random close packing generated by presented algorithm.

Supplementary Files

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