

1 **Hydromechanical State of Soil Fluidisation – A**
2 **Microscale Perspective**

3
4 **Shay Haq**

5 *BSc (Hons., Pak.), MEng (AIT)*

6 Ph.D. Candidate, School of Civil and Environmental Engineering, Faculty of Engineering and
7 IT, University of Technology Sydney (UTS), Sydney NSW 2007, Australia.

8 Email: Shay.Haq@student.uts.edu.au

9
10 **Buddhima Indraratna**

11 *BSc (Hons., Lond.), MSc (Lond.), DIC, PhD (Alberta), FTSE, FIEAust., FASCE, FGS*

12 Distinguished Professor and Director, Transport Research Centre, Faculty of Engineering and
13 IT, University of Technology Sydney (UTS), Sydney NSW 2007, Australia.

14 Email: Buddhima.Indraratna@uts.edu.au, Ph: +61 400 213 046

15
16 **Thanh Trung Nguyen**

17 *PhD (Wollongong), MEng (Saitama), BEng (Hons), CPEng, M. ASCE*

18 Research Fellow, Transport Research Centre, School of Civil and Environmental
19 Engineering, Faculty of Engineering and IT, University of Technology Sydney (UTS),
20 Sydney NSW 2007, Australia.

21 Email: thanh.nguyen-4@uts.edu.au

22 **Cholachat Rujikiatkamjorn**

23 *BEng (Hons), MEng (AIT), Ph.D. (Wollongong), FIEAust., MASCE*

24 Professor, School of Civil and Environmental Engineering, Faculty of Engineering and IT
25 University of Technology Sydney (UTS), Sydney NSW 2007, Australia.

26 Email: Cholachat.Rujikiatkamjorn@uts.edu.au

27
28 Submitted to Acta Geotechnica

29 Words: 5015

30 Figures: 14

31 Tables: 1

32

1 **Abstract**

2 This paper investigates soil fluidisation at the microscale using the Discrete Element Method
3 (DEM) in combination with the Lattice Boltzmann Method (LBM). Numerical simulations
4 were carried out at varying hydraulic gradients across the granular assembly of soil. The
5 development of local hydraulic gradients, the contact distribution, and the associated fabric
6 changes were investigated. Microscale findings suggest that a critical hydromechanical state
7 inducing fluid-like instability of a granular assembly can be defined by a substantial increase
8 in grain slip associated with a rapid reduction in interparticle contacts. Based on these
9 results, a new micromechanical criterion is proposed to characterise the transformation of
10 granular soil from a hydromechanically stable to an unstable state. The constraint ratio (ratio
11 of the number of constraints to the number of degrees of freedom) is introduced to portray
12 the relative slippage between particles and the loss of interparticle contacts within the
13 granular fabric. Its magnitude of unity corresponds to the condition of zero effective stress,
14 representing the critical hydromechanical state. In practical terms, the results of this study
15 reflect the phenomenon of subgrade mud pumping that occurs in railways when heavy-haul
16 trains pass through at certain axle loads and speeds.

17 **Keywords:** Fluidisation, Discrete Element Method, Lattice Boltzmann Method, Constraint
18 Ratio, Critical Hydraulic Gradient

19 =====

20 **1. Introduction**

21 A major problem leading to railroad instability that creates immense maintenance costs is
22 related to the degradation of the soft subgrade and its potential for fluidisation or mud-
23 pumping [1–5]. In this context, fluidisation is defined as when saturated soils are exposed to
24 excessive hydraulic gradients and lose their intergranular contacts to transform into a fluid-
25 like state. As a result, this slurry of fine particles migrates (pumps) into the overlying coarser
26 ballast layer, hence the commonly used term mud-pumping, as investigated experimentally
27 [1, 4, 6, 7]. These laboratory tests enable a better understanding of the hydromechanical
28 behaviour of the subgrade soils, but primarily at the macroscale. From a micromechanical
29 perspective, i.e., at the grain level, slippage and/or breakage of the interparticle contacts and
30 the resulting fabric evolution may initiate the transition from a hydromechanically stable to
31 an unstable state that is still not fully understood. Hydromechanically stable state means that
32 the effective stresses are still present in the soil layer to resist fluidisation. The unstable state
33 means that there are no effective stresses in the layer, and the soil has fluidised after
34 experiencing a higher number of broken contacts and zero shear resistance.

35 The Discrete Element Method (DEM) is a useful tool for assessing the micromechanics of
36 a granular medium [8, 9] that has been effectively used to study the evolution of interparticle
37 contacts and fabric during shear using the scalar and directional parameters [10–13]. In this
38 study, the scalar parameters are chosen for the purpose of analysis since the fluidisation
39 behaviour is closely related to scalar measurements of the fabric. The coordination number
40 (number of contacts per particle in the granular assembly) is a fundamental microscale fabric
41 descriptor for characterising granular medium [11, 13]. Nonetheless, the state of interparticle
42 contacts and fabric during fluid flow has rarely been considered. In addition, the constraint
43 ratio, defined by the ratio of the number of constraints to the number of degrees of freedom

44 within the particle system [14], can be used to represent the relative slip and loss of
45 interparticle contacts during instability.

46 The primary scope of this paper includes an attempt to describe and quantify the critical
47 hydromechanical conditions corresponding to the fluidisation phenomenon with special
48 attention to granular soil at the microscale, adopting the concepts of the coordination number
49 and the constraint ratio, as mentioned above. In this context, the DEM can be combined with
50 unresolved and resolved Computational Fluid Dynamics (CFD) to study fluid-particle
51 interaction in detail [15–18]. Neither of these studies could accurately quantify the critical
52 hydromechanical conditions leading to potential fluidisation from a microscale perspective,
53 so a more insightful microscale study of this instability process is needed.

54 In view of the above, this study uses a combined LBM-DEM approach that is becoming
55 increasingly popular to investigate fluid-particle interactions [19–25]. The advantages of fully
56 resolved approaches (using LBM) over unresolved approaches include (a) the ability to
57 generate a much finer mesh size, i.e., finer than the particles that can simulate true
58 experimental conditions, (b) a higher computational speed when executed on parallel
59 computers and, (c) the relative feasibility of implementation in complex geometries of porous
60 media [26, 27]. In addition, the LBM is based on the kinetic theory of gases and represents a
61 fluid through an assembly of particles that go through successive collision and propagation
62 processes. This enables the calculation of the macroscopic fluid velocity and the pressure as a
63 function of the momentum of these particles [27, 28].

64 **2. Lattice Boltzmann Method (LBM) combined with Discrete Element Method (DEM)**

65 The theoretical formulations of the LBM-DEM approach are described as follows:

66 *2.1 Fluid equations*

67 The governing Boltzmann equation is written as [29]:

$$68 \quad \frac{\partial f_\alpha(x, t)}{\partial t} + e_\alpha^v \nabla f_\alpha(x, t) = \Omega_\alpha \quad (\alpha = 1, 2, \dots, N) \quad (1)$$

69 where $f_\alpha(x, t)$ is the particle distribution function in the α direction, e_α^v is the microscopic
70 fluid velocity and Ω_α is the collision operator, and t is the time. Equation (1) can be
71 discretised on a regular lattice using a unique finite difference method, and the lattice-
72 Boltzmann equation with the Bhatnagar-Gross-Krook (BGK) collision operator for a
73 Newtonian fluid is written as [29, 30]:

$$74 \quad f_\alpha(x + e_\alpha^v \Delta t, t + \Delta t) - f_\alpha(x, t) = \Omega_\alpha^{BGK} \quad (2)$$

75 where Ω_α^{BGK} is the BGK collision operator, and Δt is the time-step.

76 Each time step is divided into two sub-steps, i.e., the collision and streaming step, and the
77 collision step is written as:

$$78 \quad f_\alpha(x, t^*) = f_\alpha(x, t) + \Omega_\alpha^{BGK} \quad (3)$$

79 $f_\alpha(x, t^*)$ and $f_\alpha(x, t)$ are the particle distribution functions after and before the collision,
80 respectively, and t^* is the time after the collision. In the streaming step, the $f_\alpha(x, t^*)$ is
81 propagated over the lattice grid as follows:

$$82 \quad f_\alpha(x + e_\alpha^v \Delta t, t + \Delta t) = f_\alpha(x, t^*) \quad (4)$$

83 *2.2 Fluid-particle interaction*

84 The participation of solid particles in the fluid is achieved by introducing an additional
85 collision term (Ω_α^s) in equation (3) [31]:

$$86 \quad f_\alpha(x, t^*) = f_\alpha(x, t) + [1 - B] \Omega_\alpha^{BGK} + B \Omega_\alpha^s \quad (5)$$

$$87 \quad B = \frac{\varepsilon_s(\tau/\Delta t - 1/2)}{(1 - \varepsilon_s) + (\tau/\Delta t - 1/2)} = (0,1) \quad (6)$$

88 where ε_s is the solid fraction in the fluid cell volume, B is a weighting function for correcting
 89 the collision phase of the lattice-BGK equation due to the presence of solid particles, and τ is
 90 the relaxation time (Appendix 1). The method for calculating the solid fraction for the
 91 moving particles is described by Seil [32].

92 The non-equilibrium part of the particle distribution function is bounced back and Ω_α^s is
 93 computed using:

$$94 \quad \Omega_\alpha^s = f_{-\alpha}(x, t) - f_\alpha(x, t) + f_\alpha^{eq}(\rho_f, v^p) - f_{-\alpha}^{eq}(\rho_f, u) \quad (7)$$

95 where v^p is the velocity of solid particle p at time $t + \Delta t$ at the node, u is the macroscopic
 96 fluid velocity, and the notation $f_{-\alpha}$ is the rebound state obtained by reversing all microscopic
 97 fluid velocities, i.e., e_α^v to $e_{-\alpha}^v$. Further details on the fluid equations and the fluid-particle
 98 interaction are described in Appendix A.

99 Figure 1 shows the flowchart of the LBM-DEM approach described above. The DEM
 100 calculation cycles are within the LBM cycles. A suitable interval for the information transfer
 101 was chosen so that the accuracy of the simulation could not be impaired. The DEM code
 102 LAMMPS Improved for General Granular, and Granular Heat Transfer Simulations
 103 (LIGGGHTS) was coupled with LBM code PALABOS [32, 33].

104 **3. Simulating Soil Specimen Fluidisation**

105 *3.1 Simulation approach*

106 Three-dimensional LBM-DEM simulations were carried out using the Hertz-Mindlin
 107 contact model (Appendix B) with the Young's modulus and the Poisson's ratio of the particles

108 as 70GPa and 0.3, respectively [11, 34]. The particle density was set to 2650 kg/m³, and the
109 rigid boundary walls were used. The most widely employed boundary type includes rigid
110 boundaries with frictional walls (O’Sullivan [9]) and they have been used in the past to
111 simulate fluidisation and internal instability (e.g., Thornton et al. [35], Nguyen and Indraratna
112 [16], Kawano et al. [36]). Based on these past studies, frictional walls as boundary conditions
113 have been adopted in this study. In a real soil column, the use of frictional walls considers the
114 presence of lateral grains. Although, periodic boundaries could have been used instead (e.g.
115 Thornton [11]). Rigid frictional boundaries are often more straightforward to implement than
116 periodic boundaries. Not examining the influence of different boundary conditions on the
117 micromechanics of the soil sample is a limitation of the current study. The gravitational
118 deposition method was used for sample preparation [37], whereby the acceleration due to the
119 force of gravity of the particles was set to 9.81 m/s². The particles were initially created in a
120 larger volume with no overlap and then dropped under gravity. The particles were allowed to
121 settle until equilibrium was reached, thereby ensuring that the coordination number remained
122 constant for a sufficient number of numerical cycles. The sample was prepared in a dense
123 state by setting the coefficient of friction (μ_s) to 0 [34, 37, 38]. Subsequently, μ_s was changed
124 to 0.30, and the particles were re-equilibrated with a sufficient number of numerical cycles
125 before the particles became saturated with the fluid [11, 38]. The μ_s value used in this study is
126 in the range of real quartz particle values that can be determined experimentally with a
127 micromechanical interparticle loading apparatus (e.g., [39]). It is assumed that the particle-
128 wall contact parameters correspond to the particle-particle contact parameters [40].

129 The fluid density was set to 1000 kg/m³ with a kinematic viscosity of 1 x 10⁻⁶ m²/s
130 according to pure water properties at 20 °C and 1 atmosphere (101 kPa). The resolution of the
131 fluid lattice was chosen with at least 5 lattices in each particle, i.e., the smallest particle
132 diameter corresponds to at least 5 fluid cells with regard to the validation of the single

133 particle displaced downwards into the fluid as described previously. A relaxation parameter
134 close to but greater than 0.50 was chosen, and the Mach number was kept below 0.1, inspired
135 by the need for improved accuracy, as explained elsewhere by Han et al, [26]. The fluid flow
136 was initiated with the relevant inlet and outlet pressure boundary conditions, and no-slip
137 conditions were imposed on the boundaries perpendicular to the flow. For each hydraulic
138 gradient applied, the flow was continued over a sufficient period of time until a steady-state
139 condition was attained. The flow was initiated in the upward direction with the gravity of the
140 particles on.

141 *3.2 Particle size distribution and homogeneity of the sample*

142 Figure 2(a) shows the particle size distribution of the selected sample from an
143 experimental study carried out by Indraratna et al. [41]. Figure 2(b) shows the three-
144 dimensional DEM-based sample with 17607 particles, and the direction of flow of the fluid is
145 also shown, i.e., the z -direction. Mud pumping and fluidisation occur owing to the upward
146 flow induced by the excessive hydraulic gradient (e.g., Indraratna et al. [7, 41]), which is why
147 the authors have chosen the z -direction (upward direction) for simulation purposes. Figure
148 2(c) shows the division of the sample into 10 different inner layers. The ratio of the lateral
149 dimension of the simulation domain to the maximum particle diameter was kept greater than
150 12 in order to obtain a representative elementary volume (REV) and avoid the boundary
151 effects. A local increase in the void ratio occurs near the rigid boundaries [9]; hence, the
152 bottom boundary layer (besides the rigid bottom boundary) was neglected in order to nullify
153 the boundary effects [42]. The thickness of each layer was chosen to be more than twice the
154 maximum particle diameter to define a REV [42]. The stresses at the boundaries do not
155 reflect the actual material response; therefore, the interaction of the particles in each layer
156 with the lateral boundaries was not taken into account.

157 Figure 2(c) shows the similar initial void ratios of all layers, indicating the REV in each
 158 layer, and the initial homogeneity of the sample was further confirmed by considering the
 159 variances in the void ratios as reported by Jiang et al. [43]:

$$160 \quad S^2 = \frac{1}{n_L - 1} \sum_{k=1}^{n_L} (e_{oi}^k - e_{oi}^{avg})^2 \quad (8)$$

161 where S is the variance of the void ratios, n_L is the total number of layers, e_{oi}^k is the initial
 162 void ratio of the k^{th} layer, and e_{oi}^{avg} is the initial void ratio of the entire sample. The S^2 value
 163 for the sample in Fig. 2(c) is 2.72×10^{-5} , which is sufficiently low to classify the sample as
 164 homogenous with respect to the REV in each layer. The overall void ratio of the numerical
 165 sample is the same as that of the experimental sample. Note that the void ratio does not take
 166 into account the particulate structure of the granular medium. Figure 2(d) shows a close-up
 167 view of the particles modelled in the fluid mesh. It can be seen that the mesh size is much
 168 smaller than the particle and pore size, in contrast to the conventional unresolved approach
 169 with the Navier-Stokes equation.

170 3.3 Calibration

171 Fluid and grain densities were determined from previous experimental investigations
 172 carried out earlier by the authors (Indraratna et al. [41]), and the contact friction angle was
 173 chosen from previous DEM studies on similar granular materials (e.g., Sufian et al. [44]).
 174 Since the above parameters were determined at the initial stage, the relaxation time (τ) was
 175 then obtained during the calibration process. Figure 3a shows the calibration of the relaxation
 176 time (τ) for soil fluidisation by comparing the pressure drops obtained from the LBM-DEM
 177 approach and an analytical solution (Ergun [45]). For further analysis, a relaxation time (τ) =
 178 0.56 was chosen, and this is in line with the appropriate value of the kinematic viscosity of
 179 the water as used in the experiments. Figure 3b compares the flow curves obtained from the

180 LBM-DEM approach and an earlier experimental study [41]. The flow curves obtained from
 181 the LBM-DEM approach and experimental methods agree. The overall critical hydraulic
 182 gradient ($i_{o,cr}$) refers to the gradient at which the effective stresses drop to zero, and the soil
 183 becomes fluidised. $i_{o,cr}$ predicted by the LBM-DEM approach was 1.050, while the
 184 experimental value of $i_{o,cr}$ was 1.180. These values are in reasonable agreement with each
 185 other. This acceptable agreement with the experimental results implies that the lattice
 186 resolution of 5 fluid cells per particle is sufficient to capture the fluidisation behaviour of the
 187 particle size distribution considered in this study. Nevertheless, in complex LBM-DEM
 188 modelling such as this, where a huge number of particles of different sizes and shapes cannot
 189 be accommodated to represent an ideal real-life pore structure or void distribution due to the
 190 obvious computational challenges, one cannot guarantee perfect accuracy; this is recognised
 191 as a current limitation to be further improved in the future.

192 **4. Results and Discussion**


193 *4.1 Stress-hydraulic gradient evolution*

194 Figure 4a shows the evolution of overall hydraulic gradient over time. Figure 4b shows the
 195 stress-hydraulic gradient space where the local hydraulic gradients (i_{hyd}) are plotted against
 196 the normalised Cauchy effective stresses ($\sigma'_{zz}/\sigma'_{zz0}$) of particles in a given layer in the fluid
 197 flow direction (vertical direction) at any time, where σ'_{zz} is the Cauchy effective stresses of
 198 the particles in a layer at any time, and σ'_{zz0} is the initial Cauchy effective stresses of the
 199 particles in that particular layer. The σ'_{zz} is obtained using the particle-based stresses via the
 200 following second-order stress tensor equation [46].

$$201 \quad \sigma'_{ij} = \frac{1}{V} \sum_{p=1}^{N_p} \sigma_{ij}^{p'} V^p \quad (9)$$

202 where V is the volume of the layer or the selected region, V^p is the volume of particle p in the
 203 region, N_p is the number of particles in the layer, and $\sigma_{ij}^{p'}$ is the average stress tensor within a
 204 particle p and is given by:

$$205 \quad \sigma_{ij}^{p'} = \frac{1}{V^p} \sum_{c=1}^{N_c^p} |x_i^c - x_i^p| n_i^{c,p} f_j^c \quad (10)$$

206 where f_j^c is the force vector in the j^{th} direction at contact c with the location x_i^c , x_i^p is the
 207 location of the particle's centroid, $n_i^{c,p}$ is the unit normal vector from the particle's centroid to
 208 the contact location and N_c^p is the number of contacts on the particle p . Note that equations
 209 (9) and (10) compute the effective stresses directly from the contact moments and not
 210 according to Terzaghi's concept used in the macroscale laboratory studies. Reynold's stresses
 211 are negligible and are not taken into account. 

212 Figure 4b shows that the onset of fluidisation of the soil is associated with hydraulic and
 213 stress conditions, i.e., hydromechanical conditions. The effective stresses decrease with
 214 increasing local hydraulic gradients in each layer. The onset occurs at a critical hydraulic
 215 gradient when the effective stresses drop to zero. The evolution of the stress-gradient of each
 216 layer is not the same. The stress-gradient paths of Layers 1-6 are approximately linear with a
 217 slope of -1. In contrast to the theoretical linear stress-gradient paths presented by Li and
 218 Fannin (2012), the stress-gradient paths of Layers 7-10 (lower layers) are nonlinear until
 219 failure. The failure initiates when the effective stress of Layer 10 approaches zero. At the
 220 same time, Layers 1-9 show residual stresses due to the motion of the particles in the form of
 221 clusters. These residual stresses decrease as the particles in the cluster would lose further
 222 contacts over time after onset until complete fluidisation occurs.

223 Lateral (horizontal) stresses did not affect fluidisation in the current study, as the ratio
224 between the horizontal and vertical stresses was always less than 1 at the hydrostatic state and
225 before fluidisation (see Figures 5a and 5b). The effective horizontal stresses (due to increased
226 water pressure) decrease to zero, so it is the vertical stresses that predominantly control the
227 onset of fluidisation (Figure 5b). In this respect, there is no possibility of any arching effect
228 when approaching the state of fluidisation, and only the vertical stresses should be considered
229 when quantifying soil fluidisation. In real-life situations, the observed instability of shallow
230 soil deposits (e.g., mud pumping under cyclic train loading) has also proven that the ratio of
231 effective lateral to vertical stresses in the field is smaller than unity.

232 4.2 Broken contacts

233 Figure 6 shows the development of the broken contacts (B_R) compared to the normalised
234 effective stresses ($\sigma'_{zz}/\sigma'_{zz0}$). B_R is the percentage of interparticle contact losses in the initial
235 number of contacts in the corresponding layer. The value of B_R increases with increasing
236 hydraulic gradient and decreasing effective stresses. Contact is lost when the normal contact
237 force due to hydrodynamic forces becomes zero. When the fluid flows, the contacts break off,
238 and new contacts are also formed in the layer. The sharp turn in B_R represents the critical
239 hydromechanical state where the contacts are notably lost. The granular assembly would
240 become a fully fluid-like material when the number of unconnected particles increases to the
241 maximum due to the breakage of the contacts, i.e., most of the particles would simply float
242 without any contact. It can also be seen that the contact losses in the lower layers are greater
243 than in the upper layers, which shows that more particles lose contact at the bottom and
244 migrate upwards with the fluid flow if the constrictions are wide enough. The B_R at the
245 critical hydraulic gradient is about 5% in Layer 1 and 17% in Layer 10 and increases
246 considerably with a further slight increase in the hydraulic gradient applied across the soil
247 specimen. The bottom layer has a higher percentage of broken contacts because the local

248 hydraulic gradient is higher in the bottom layer than in the top layer. This difference in local
249 hydraulic gradients is attributed to anisotropy in the contact and pore networks due to gravity
250 deposition. The microscale parameters considered in this study can be determined in the field
251 where the variations in hydraulic gradients, effective stresses and void ratios can be
252 predicted, and then used to back-calculate these microscale parameters.

253 *4.3 Mechanically stable particles*

254 Figure 7 shows the evolution of the fraction of mechanically stable particles (M_s) with
255 normalised effective stresses ($\sigma'_{zz}/\sigma'_{zz0}$) under increasing hydraulic gradients. The
256 mechanically stable particles are those that participate in the stable network of force
257 transmission. The value of M_s is defined by [48]:

$$258 \quad M_s = \frac{N_p^{\geq 4}}{N_p} \quad (11)$$

259 where $N_p^{\geq 4}$ is the number of particles with at least 4 or more contacts. Particles with zero
260 contacts that do not participate in the stable network of force transmission are called rattlers
261 or unconnected particles; hence, they are excluded. The particles with 1, 2, and 3 contacts are
262 temporarily stable for a limited time, so they are also neglected in the above equation.

263 It should be noted that the values of M_s are always smaller than 1 across all layers since
264 the temporarily stable particles are also present at the hydrostatic state. The initial values of
265 M_s are higher in the lower layers than in the upper layers. The values of M_s decrease across
266 all layers with a decrease in the values of the effective stresses. This reduction becomes
267 significant at the critical hydraulic and stress conditions that indicate the breakup of the
268 clusters of mechanically stable particles. The results show that a critical value of $M_s \approx 0.75$ is
269 found for all layers, below which the fluid-like behaviour of the soil is observed.

270 4.4 Evolution of the soil fabric

271 Figure 8 shows a conceptual model that describes the differences in the fabrics of two-
272 particle systems where particles with two different geometrical arrangements are placed. Note
273 that the void ratios of both arrangements are the same. However, the number of interparticle
274 contacts is different due to the dissimilarity of the fabrics of the particulate systems. It is
275 noteworthy that the geometric arrangement of the particles is more important than the void
276 ratio when it comes to the strength of the granular assembly [14]. Similar initial void ratios of
277 all layers indicate that the number of particles in each layer is the same. However, the number
278 of interparticle contacts can vary due to the different geometrical configurations of the
279 particles. During fluid flow, the number of particles in each layer remains unchanged until
280 fluidisation begins, while the geometrical re-arrangement of the particles can occur, mainly
281 due to the fact that the interparticle contacts within the layer slip and/or break.

282 To assess the evolution of soil fabric under fluid flow, this study uses a scalar approach
283 (e.g., Fonseca et al., 2013) to quantify the fabric with a scalar fabric descriptor called the
284 coordination number (Z) and is computed as follows [11].

$$285 \quad Z = \frac{2N_c}{N_p} \quad (12)$$

286 where N_c is the number of contacts and is multiplied by 2 since each contact is shared by two
287 different particles. The coordination number is a basic descriptor to quantify the fabric, and
288 the non-application of more advanced approaches is a limitation of this study.

289 Figure 9 shows the distribution of the Z at the hydrostatic state and the onset of soil
290 fluidisation, taking into account three distinct cases:

291 (a) all particles

292 (b) particles with diameters (d_p) $\geq d_{50}$ (where d_{50} is the particle size that is 50% finer by
293 mass), and

294 (c) particles with $d_p \geq d_{85}$ (where d_{85} is the particle size that is 85% finer by mass)

295 Despite the narrow range in the particle size distribution curve, the difference in the
296 coordination number distribution becomes clearer when the conditions $d_p > d_{50}$ and $d_p > d_{85}$
297 are applied. Therefore, it is essential to consider all cases.

298 Figure 9(a) shows that the distribution of the coordination numbers at the hydrostatic state
299 across different layers is somewhat dissimilar when all particles are considered. This
300 difference is enhanced when the larger particle sizes are taken into consideration (Figures
301 9(c) & 9(e)), which shows a dissimilarity in the fabric of all layers despite the similar void
302 ratios. This fabric dissimilarity is ascribed to the influence of gravity during the sample
303 preparation phase. The curves of the lower layers are on the right-hand side and show higher
304 values of the coordination numbers than those of the upper layers. The slight difference in the
305 evolution of local hydraulic gradients and effective stresses through each layer, as previously
306 described, is due to this slight dissimilarity of the particles' fabric in the layers. It is appealing
307 to note that at the onset of fluidisation, the distributions of the coordination numbers of all
308 layers converge and become similar (Figures 9(b), 9(d), & 9(f)). The median value of the
309 coordination number (Z_{50}) is 4 when all particles in the granular medium of the layer are
310 taken into account (Figure 8(b)). Thus, at the onset of fluidisation, the distributions of the
311 interparticle contacts are uniform and show a similar fabric for all soil layers.

312 Figure 10 shows average coordination numbers (Z_{avg}) versus normalised effective stresses
313 ($\sigma'_{zz}/\sigma'_{zz0}$), where the initial (at the hydrostatic state) average coordination of Layer 10 is the
314 highest (i.e., $Z_{avg} = 5.405$), while Layer 1 has the lowest (i.e., $Z_{avg} = 4.811$). As the normalised
315 effective stresses decrease, the values of Z_{avg} decrease across all layers, and so does the

316 difference between them. Although each layer initially had a different fabric, the Z_{avg} of all
317 layers has evolved to become the same, i.e., 4.6 at critical hydromechanical state.

318 4.5 Sliding index

319 Figure 11 shows the distribution of the sliding index (S_i) of the selected Layer 10. Note
320 that all layers show an almost similar development in the sliding index as the local hydraulic
321 gradient increases. The sliding index (S_i) is defined by [48]:

$$322 \quad S_i = \frac{f^T}{\mu_s f^N} \quad (13)$$

323 Sliding or the plastic contacts occur when the tangential contact force (f^T) has fully
324 mobilised the friction, i.e., $S_i = 1$. The contacts with $S_i < 1$ are the elastic contacts and f^T is
325 independent of f^N in such contacts. Note that contacts that have already been lost are not
326 taken into account when calculating S_i .

327 The results show that a small proportion of the contacts slide even at the hydrostatic state
328 since the static buoyancy forces would be acting on the particles when they are saturated with
329 the fluid. As the local hydraulic gradients increase, the elastic contacts decrease, and the
330 sliding contacts increase. The hydrodynamic forces from the seepage flow tend to move the
331 particles, causing a change in the magnitudes of the resisting tangential contact force and the
332 normal contact force. As a result, a slip is caused when the elastic tangential contact force
333 reaches the Coulomb cut-off, i.e., $f^T = \mu_s f^N$. Two types of contact networks are present,
334 strong and weak contacts. Strong and weak contact forces are defined for each layer with
335 respect to the mean contact force in each corresponding layer. The strong contacts that carry
336 the primary load are those with above-average normal contact forces; otherwise, they
337 correspond to weak contacts (Thornton and Antony [49]), and this sliding of the particles
338 occurs in the weak contacts [50]. At $i_{hyd} \leq 1$, the proportion of sliding contacts in the total

339 number of contacts in the layer is $\leq 10\%$, while it is around 17% at the critical $i_{hyd} = 1.251$
 340 (Figure 11(g)). Thereafter, this proportion of sliding contacts increases steeply with a further,
 341 albeit slight, increase in the hydraulic gradient. It is noteworthy that the maximum tangential
 342 force is controlled by the value of μ_s . Therefore, the value of μ_s has a profound influence on
 343 the proportion of sliding contacts and consequently on the macroscale behaviour of the
 344 granular assembly.

345 4.6 Constraint ratio

346 Figure 12 shows a three-dimensional representation of the constraint ratio (R) versus local
 347 hydraulic gradients (i_{hyd}) and normalised effective stresses ($\sigma'_{zz}/\sigma'_{zz0}$). The constraint ratio for
 348 a three-dimensional particle system that only takes the sliding resistance into account is given
 349 by [14]:

$$350 \quad R = \frac{N_{ct}}{N_d} = \frac{N_c(3 - 2S_c)}{6N_p} \quad (14)$$

351 where N_{ct} is the number of constraints, N_d is the number of degrees of freedom, and S_c is the
 352 fraction of slipping contacts in the total number of contacts at a given point in time. For an
 353 idealised granular medium with $\mu_s = \infty$, $N_{ct} = 3N_c$ and $N_d = 6N_p$. The realistic granular
 354 medium, however, would have a finite value of μ_s ; therefore, the two tangential force
 355 constraints on contacts subject to slipping vanish and are excluded from the total number of
 356 constraints given in equation (14). Theoretically, if $N_{ct} > N_d$, the granular assembly is
 357 considered to be over-constrained or mechanically stable, and if $N_{ct} = N_d$, it is considered to
 358 be in a critical or transitional state; otherwise, it is unstable. Note that R represents both
 359 slipping and loss of contacts in the particle systems, whereas the coordination number [11]
 360 does not take into account the slipping of particles.

361 The constraint ratio in each layer decreases according to the nonlinear power laws when
362 the normalised effective stresses decrease, and it decays exponentially after the onset of the
363 soil fluidisation (Fig. 12). The initial mild slope shows that at the relatively low i_{hyd} values,
364 i.e., $i_{hyd} < 1$, the particles slip less and have minimal loss of contacts. The abrupt change in
365 slope after onset is triggered by substantial slipping and the associated rapid loss of
366 interparticle contacts. The point at which the slope value changes represents the critical
367 microscale hydromechanical state or the onset of soil fluidisation. This point is marked as a
368 transition line from a hydromechanically stable to a fluid-like state, as shown in Fig. 12(b).
369 This critical hydromechanical state corresponds to $R \approx 1$, with effective stresses ≈ 0 at the
370 critical hydraulic gradient. Therefore, the soil is hydromechanically stable when R is greater
371 than 1. It is in a transition state from a hydromechanically stable to a fluid-like state when R
372 is 1; otherwise, it corresponds to a slurry or fluid-like state. Complete fluidisation of the soil
373 specimen occurs when almost all interparticle contacts are lost, with a constraint ratio well
374 below 1.

375 5. Conclusions

376 This study assessed the hydromechanical state of soil fluidisation from a
377 micromechanical perspective using the LBM-DEM approach. The good agreement between
378 the model predictions and the experimental observations in relation to particle motion, fluid
379 flow curves, and the critical hydraulic gradients confirms the capability and reliability of this
380 hybrid numerical method. Based on the findings of this study, the following salient outcomes
381 can be drawn:

- 382 • At comparatively low values of the local hydraulic gradient (i_{hyd}), i.e., $i_{hyd} \leq 1$, the
383 proportion of slipping contacts in the total number of contacts of the selected Layer 10
384 (bottom of the specimen) was $\leq 10\%$, while it was approximately 17% at the critical i_{hyd}

385 =1.251. The extent of slipping contacts increased with a further increase in the hydraulic
386 gradient applied across the soil specimen.

387 • The fraction of mechanically stable particles was generally larger at the deeper layers but
388 decreased with the reduction in normalised effective stress during the corresponding
389 increase in hydraulic gradient. The fluid-like state of soil was triggered when this fraction
390 of mechanically stable particles dropped below 0.75.

391 • The hydrodynamic forces induced by the seepage flow inevitably destabilize and move
392 the particles within the granular assembly, resulting in reduced contact forces, thus
393 creating critical conditions to facilitate particle slipping. The loss of interparticle contacts
394 was not uniform across the depth of the soil specimen, as this was more pronounced in
395 the deeper layers when subjected to an upward flow from the base of the specimen.

396 • At the critical hydraulic gradient, the percentage of interparticle contact losses relative to
397 the initial number of contacts was non-uniform and varied between 5 and 17% across the
398 specimen depth. After that, even with a slight increase in the hydraulic gradients, the
399 breakage of the interparticle contacts appeared to exacerbate.

400 • At the onset of fluidisation, the distributions of the coordination numbers across all layers
401 of the soil specimen became more uniform, with a median value of 4 and an average
402 value of 4.6, thus representing a more uniform granular fabric across the soil layers.

403 • The constraint ratio (ratio of the number of constraints to the number of degrees of
404 freedom in the particle system) was used to distinguish hydromechanically stable and
405 unstable states. A value of the constraint ratio greater than 1 represented the
406 hydromechanically stable state and less than 1 the unstable state. The critical
407 hydromechanical state was found at a constraint ratio of unity. Constraint ratio
408 represented the slippage and loss of contacts in the particle system, and its value
409 decreased with the increase in the hydraulic gradient. The slipping and the associated loss

410 of contact between the soil particles would cause the effective stresses to drop. This
411 implies from a microscale perspective that soil fluidisation could be triggered by
412 excessive slippage and the inevitable loss of contacts between particles.

413 **Declaration of Competing Interest**

414 The authors state that they are not aware of any competing financial interests or personal
415 relationships that may have influenced the work reported in this paper.

416 **Acknowledgements**

417 The financial support from the Transport Research Centre, University of Technology Sydney,
418 Sydney, Australia, is expressly recognised.

419 **Data availability statement**

420 The data will be made available by the authors upon reasonable request.

421 **Appendix A. LBM-DEM Approach**

422 The Ω_α^{BGK} , through which the momentum transfer occurs between the fluid particles
423 when they collide, is given by [30]:

$$424 \quad \Omega_\alpha^{BGK} = -\frac{\Delta t}{\tau} \left(f_\alpha(x, t) - f_\alpha^{eq}(x, t) \right) \quad (A.1)$$

425 where $f_\alpha^{eq}(x, t)$ is the equilibrium distribution function, τ is the relaxation time, and is related
426 to the kinematic viscosity (ν_f) of the fluid, the lattice spacing (Δx), and the time step (Δt) by
427 the following relationship:

$$428 \quad \nu_f = \frac{1}{3} \left(\tau - \frac{1}{2} \right) \frac{\Delta x^2}{\Delta t} \quad (A.2)$$

429 Equation (A.2) implies that the τ value should be greater than 0.5. For a given value of v_f
 430 and τ , the Δt is defined according to the chosen Δx by:

$$431 \quad \Delta t = \frac{1}{3v_f} \left(\tau - \frac{1}{2} \right) \Delta x^2 \quad (A.3)$$

432 The $f_\alpha^{eq}(x, t)$ for the BGK model is given by [30]:

$$433 \quad f_\alpha^{eq}(x, t) = \omega_\alpha \rho_f \left(1 + \frac{3}{c_L^2} e_\alpha^v u + \frac{9}{2c_L^4} (e_\alpha^v u)^2 - \frac{3}{2c_L^2} u^2 \right) \quad (A.4)$$

434 where, ω_α is the weighting factor for the velocity vectors, ρ_f is the fluid density, e_α^v is the
 435 microscopic fluid velocity, u is the macroscopic fluid velocity, and c_L is the lattice speed
 436 given by:

$$437 \quad c_L = \frac{\Delta x}{\Delta t} \quad (A.5)$$

438 In lattice Boltzmann computations, $c_L = \Delta x = \Delta t = 1$, and the discretisation schemes in
 439 LBM are labelled as $DdQq$, where d is the number of dimensions, and q represents the
 440 number of velocity vectors. This study used the $D3Q19$, a three-dimensional scheme with 19
 441 velocity vectors, including one at rest. Figure A.1 shows the directions of the velocity vectors
 442 (e_α^v) for the $D3Q19$ scheme and, for the sake of simplicity, their magnitudes are already
 443 defined by:

$$444 \quad e_\alpha^v = \begin{cases} (0,0,0) & i = 0 \\ (\pm c_L, 0,0), (0, \pm c_L, 0), (0,0, \pm c_L) & i = 1,2,3,4,5,6 \\ (\pm c_L, \pm c_L, 0), (\pm c_L, 0, \pm c_L), (0, \pm c_L, \pm c_L) & i = 7,8,9,10,11, \dots, 18 \end{cases} \quad (A.6)$$

445 and the weighing factors are $\omega_0 = 1/3$, $\omega_{1,2,3,4,5,6} = 1/18$ and $\omega_{7,8,\dots,18} = 1/36$.

446 The macroscopic fluid properties, i.e., fluid density (ρ_f) and velocity (u) can be retrieved
 447 at each node and given by (Han & Cundall, 2017; Seil et al., 2018):

448
$$\rho_f(x, t) = \sum_{\alpha=0}^{q-1} f_{\alpha}(x, t) \quad (A.7)$$

449
$$u(x, t) = \frac{1}{\rho_f} \sum_{\alpha=0}^{q-1} f_{\alpha}(x, t) e_{\alpha}^v \quad (A.8)$$

450 To determine the fluid pressure p_f , it is assumed that the fluid is slightly compressible, and
 451 the following state equation is used:

452
$$p_f = c_s^2 \rho_f \quad (A.9)$$

453 where c_s is the sound celerity and is defined by:

454
$$c_s = \frac{c_L}{\sqrt{3}} \quad (A.10)$$

455 Fluid modelled with LBM requires a slight variation in spatial density. An approximate
 456 incompressibility situation can only be achieved under the condition that the Mach number
 457 (M) is small; is therefore kept below 0.1 [26], and is defined by:

458
$$M = \frac{u_{max}}{c_L} \quad (A.11)$$

459 u_{max} is the maximum velocity in the fluid flow in physical units. Fluids with lower viscosity
 460 and turbulent flows can also be simulated with LBM using the Smagorinsky Large Eddy
 461 Simulation approach [28, 51]. Unit conversion between physical and lattice units is explained
 462 elsewhere by Latt [52].

463 For the fluid-particle interaction, the force (f_f) (without the static buoyancy force) and the
 464 torque (T_f) acting on a particle through the fluid can then be computed by [28, 31]:

465
$$f_f = \frac{\Delta x^3}{\Delta t} \left[\sum_n B_n \sum_\alpha \Omega_\alpha^s e_\alpha^v \right] \quad (A.12)$$

466
$$T_f = \frac{\Delta x^3}{\Delta t} \left[\sum_n B_n (x^n - x^p) \sum_\alpha \Omega_\alpha^s e_\alpha^v \right] \quad (A.13)$$

467 B_n is the weighting function in the cell, x^n is the coordinate of the lattice cell, and x^p is the
 468 centre of mass of the particle. Equation (A.12) does not include the static buoyancy forces;
 469 therefore, they are applied separately to the particles and the total hydrodynamic force (f_{hyd})
 470 on the particle, including the static buoyancy force (f_{bu}) is given by:

471
$$f_{hyd} = f_f + f_{bu} \quad (A.14)$$

472 The governing equations of motion of solid particles given by Cundall & Strack (1979),
 473 with the additional fluid-particle interaction force and the torque, are as follows:

474
$$m^p \frac{dv^p}{dt} = f_g^p + f_{hyd}^p + \sum_{c=1}^{N_c^p} f_j^c \quad (A.15)$$

475
$$I^p \frac{dw^p}{dt} = T_f^p + \sum_{c=1}^{N_c^p} T_j^c \quad (A.16)$$

476 where m^p and I^p are the mass and the moment of inertia of the particle p , v^p and w^p are the
 477 translational and angular velocities of the particle p , N_c^p is the total number of contacts on the
 478 particle p , f_j^c is the contact force vector in the j^{th} direction at contact c on the particle p , T_j^c is
 479 the torque that acts on the particle p due to the tangential contact force at contact c , and f_g^p is
 480 the gravitational force on the particle p .

481 *A.1 Validation*

482 Although LBM-DEM was previously validated by Indraratna et al. [21] with experimental
483 observations of fluidisation, the transient motion of the particles in the fluid could not be
484 quantified. In this regard, an attempt is made in this study to validate the motion of a single
485 particle falling into the fluid with different particle Reynold's numbers (Re_p). This validation
486 is carried out by comparing the numerical results with the experimental observations by Ten
487 Cate et al. [53]. Figures A.2(a) and A.2(b) show the schematic sketch and the modelled
488 problem using the LBM-DEM approach, respectively. Table 1 shows the fluid properties
489 used with lattice resolution (N) = 5 (particle diameter corresponds to 5 fluid cells) and the
490 relaxation time (τ) = 0.53. It is noteworthy that $N = 5$ was chosen after a preliminary
491 sensitivity analysis in which the simulation was run with $N = 5, 7$ and 10. The results showed
492 insignificant difference in the numerical output when $N > 5$. Figures A.2(c) and A.2(d) show
493 an excellent agreement between the numerical and experimental results of the position and
494 velocity of the falling particle over time at different Reynold's numbers. Hence, it could be
495 justified with confidence that the LBM-DEM approach would reasonably predict the transient
496 motion of the particles in the fluid with these selected numerical parameters, i.e., $N = 5$ and τ
497 = 0.53.

498 **Appendix B. Hertz-Mindlin Contact Model**

499 Figure B.1 shows the rheological scheme and schematic sketch of the Hertz-Mindlin
500 contact model used in this study to simulate the fluidisation of the soil. The normal contact
501 force (f^N) is based on Hertzian contact theory and the tangential contact force (f^T) is based
502 on the work of Mindlin & Deresiewicz [54]. The f^N and f^T have the nonlinear spring and
503 damping components. The normal and tangential damping coefficients (c_n and c_t) are related
504 to the restitution coefficient as reported by Tsuji et al. [55]. The tangential frictional force
505 follows Coulomb's law of friction (e.g., [8]).

506 $f^N = k_n \delta_n - c_n v_n^{rel}$ (B.1)

507 where k_n is the elastic constant for normal contact, c_n is the viscoelastic damping constant
 508 for normal contact, δ_n is the normal component of the displacement at the contact as
 509 represented by the overlap distance, v_n^{rel} is the normal component of the relative velocity of
 510 two spherical particles, and k_n is given by:

511 $k_n = \frac{4}{3} E^* \sqrt{R^* \delta_n}$ (B.2)

512 where E^* is the equivalent Young's modulus and R^* is the equivalent radius which can be
 513 written as follows:

514 $\frac{1}{R^*} = \frac{1}{R_i} + \frac{1}{R_j}$ (B.3)

515 $\frac{1}{E^*} = \frac{1 - \nu_i^2}{E_{y_i}} + \frac{1 - \nu_j^2}{E_{y_j}}$ (B.4)

516 where R_i and R_j are the radius, E_{y_i} and E_{y_j} are Young's modulus, and ν_i and ν_j are the
 517 Poisson's ratio of each neighbouring spheres in contact. The viscoelastic damping constant
 518 (c_n) is given by:

519 $c_n = -2 \sqrt{\frac{5}{6}} \beta \sqrt{S_n m^*} \geq 0$ (B.5)

520 where, m^* is the equivalent mass and is given by:

521 $\frac{1}{m^*} = \frac{1}{m_i} + \frac{1}{m_j}$ (B.6)

522 β and S_n are given by:

523
$$\beta = \frac{\ln e_r}{\sqrt{\ln^2 e_r + \pi^2}} \quad (\text{B.7})$$

524
$$S_n = 2E^* \sqrt{R^* \delta_n} \quad (\text{B.8})$$

525 where e_r is the coefficient of restitution. The tangential contact force (f^T) is given by:

526
$$f^T = k_t \delta_t - c_t v_t^{rel} \quad (\text{B.9})$$

527 where k_t is the elastic constant for tangential contact, c_t is the viscoelastic damping constant
 528 for tangential contact, δ_t is the tangential overlap, and v_t^{rel} is the tangential component of the
 529 relative velocity of two spherical particles, and k_t is given by:

530
$$k_t = 8G^* \sqrt{R^* \delta_n} \quad (\text{B.10})$$

531 with G^* as the equivalent shear modulus, and c_t is written as follows:

532
$$c_t = -2 \sqrt{\frac{5}{6}} \beta \sqrt{k_t m^*} \geq 0 \quad (\text{B.11})$$

533 The f^T is limited by:

534
$$f^T = \mu_s f^N \quad (\text{B.12})$$

535 where μ_s is the coefficient of sliding friction.

536 NOTATIONS

537 *The following symbols are used in this paper:*

538 B = weighing function to correct the collision phase due to the presence of solid particles,

539 B_R = percentage of broken contacts,

540 c_L = lattice speed,

541 c_n = viscoelastic damping constant for normal contact,

542 c_s = sound celerity,

543 c_t = viscoelastic damping constant for tangential contact,

544 d_p = diameter of the particle,

545 d_{50} = particle size that is 50% finer by mass in the particle size distribution,

546 d_{85} = particle size that is 85% finer by mass in the particle size distribution,

547 E^* = equivalent Young's modulus,

548 e_α^v = microscopic fluid velocity,

549 e_{oi}^k = initial void ratio of the k^{th} layer,

550 e_{oi}^{avg} = initial void ratio of the entire sample considering all 10 Layers,

551 e_r = coefficient of restitution,

552 f_{bu} = static buoyancy force on the particle,

553 f_{hyd}^p = total hydrodynamic force (including the static buoyancy force) on the particle p ,

554 f_f = hydrodynamic forces on the particle without buoyancy force,

555 f_g^p = gravitational force on the particle p ,

556 f_j^c = force vector in j^{th} direction at contact c ,

557 f^T = tangential contact force,

558 f^N = normal contact force,

559 $f_\alpha(x, t)$ = particle distribution function,

- 560 $f_{\alpha}(x, t^*)$ = particle distribution function after the collision of fluid particles,
- 561 $f_{\alpha}^{eq}(x, t)$ = equilibrium distribution function,
- 562 G^* = equivalent shear modulus,
- 563 I^p = moment of inertia of the particle p ,
- 564 i_o = overall applied hydraulic gradient,
- 565 $i_{o,cr}$ = critical overall hydraulic gradient of the soil specimen,
- 566 i_{hyd} = local hydraulic gradient in a layer,
- 567 k_n = elastic constant for normal contact,
- 568 k_t = elastic constant for tangential contact,
- 569 L = height of the particle bed,
- 570 M = Mach number,
- 571 M_s = fraction of mechanically stable particles,
- 572 m^p = mass of the particle p ,
- 573 m^* = equivalent mass,
- 574 N = lattice resolution,
- 575 N_c = number of contacts,
- 576 N_d = number of degrees of freedom,
- 577 N_{ct} = number of constraints,
- 578 N_c^p = number of contacts on particle p ,
- 579 N_p = number of particles,
- 580 $N_p^{\geq 4}$ = number of particles with at least 4 or more contacts,
- 581 n = overall porosity of the soil specimen,
- 582 $n_i^{c,p}$ = unit-normal vector from the particle' centroid to the contact location,
- 583 n_L = number of layers,
- 584 O_i = initial centroidal location of particle i ,

- 585 O_j = initial centroidal location of particle j ,
- 586 O'_j = displaced centroidal location of particle j ,
- 587 R = constraint ratio for a three-dimensional particle system with only sliding resistance,
- 588 R^* = equivalent radius,
- 589 Re_p = Reynold's number of the particle,
- 590 S = variance in the void ratios,
- 591 S_i = slipping index,
- 592 S_c = fraction of slipping contacts,
- 593 T_f^p = fluid-particle interaction torque,
- 594 T_j^c = interparticle contact torque due to tangential force,
- 595 t = time,
- 596 t^* = time after the collision,
- 597 u = macroscopic fluid velocity,
- 598 u_{max} = maximum velocity of the fluid flow in physical units,
- 599 V = volume of the selected region or layer,
- 600 V^p = volume of particle p ,
- 601 v_d = superficial or discharge velocity of the fluid,
- 602 ν_f = kinematic viscosity of fluid,
- 603 v_n^{rel} = normal component of the relative velocity of two spherical particles,
- 604 v_t^{rel} = tangential component of the relative velocity of two spherical particles,
- 605 v^p = translational velocity of the particle p ,
- 606 w^p = angular velocity of the particle p ,
- 607 ω_α = weighing factor for the microscopic fluid velocity,
- 608 x^n = coordinate of the lattice cell,

- 609 x_i^p = centre of mass of the particle,
- 610 z = location of the particle,
- 611 Z = coordination number,
- 612 $Z_{avg.}$ = average coordination number,
- 613 ΔP = pressure drop across the particle bed,
- 614 Δx = lattice spacing,
- 615 ρ_f = fluid density,
- 616 δ_n = normal overlap,
- 617 δ_t = tangential overlap,
- 618 Ω_α = collision operator,
- 619 Ω_α^{BGK} = collision operator of the BGK model,
- 620 Ω_α^s = additional collision term for solid fraction,
- 621 ε_s = solid fraction in the fluid cell volume,
- 622 τ = relaxation time,
- 623 μ_s = coefficient of sliding friction,
- 624 μ_f = dynamic viscosity of the fluid,
- 625 σ'_{ij} = Cauchy effective stress tensor in the selected region,
- 626 $\sigma_{ij}^{p'}$ = average stress tensor within a particle p ,
- 627 σ'_{zz} = Cauchy effective stresses of the particles in a layer in the fluid flow direction at any time,
- 628 and
- 629 σ'_{zzo} = initial Cauchy effective stresses of the particles in a layer in the fluid flow direction.

630 **REFERENCES**

- 631 1. Indraratna B, Singh M, Nguyen TT, et al (2020) Laboratory study on subgrade
632 fluidization under undrained cyclic triaxial loading. *Can Geotech J* 57:1767–1779.
633 <https://doi.org/10.1139/cgj-2019-0350>
- 634 2. Chawla S, Shahu JT (2016) Reinforcement and mud-pumping benefits of
635 geosynthetics in railway tracks: Model tests. *Geotext Geomembranes* 44:366–380.
636 <https://doi.org/10.1016/j.geotextmem.2016.01.005>
- 637 3. Hudson A, Watson G, Le Pen L, Powrie W (2016) Remediation of Mud Pumping on a
638 Ballasted Railway Track. *Procedia Eng* 143:1043–1050.
639 <https://doi.org/10.1016/j.proeng.2016.06.103>
- 640 4. Duong TV, Cui YJ, Tang AM, et al (2014) Investigating the mud pumping and
641 interlayer creation phenomena in railway sub-structure. *Eng Geol* 171:45–58.
642 <https://doi.org/10.1016/j.enggeo.2013.12.016>
- 643 5. Nguyen TT, Indraratna B, Kelly R, et al (2019) Mud pumping under railtracks:
644 Mechanisms, assessments and solutions. *Aust Geomech J* 54:59–80
- 645 6. Arivalagan J, Rujikiatkamjorn C, Indraratna B, Warwick A (2021) The role of
646 geosynthetics in reducing the fluidisation potential of soft subgrade under cyclic
647 loading. *Geotext Geomembranes*. <https://doi.org/10.1016/j.geotextmem.2021.05.004>
- 648 7. Indraratna B, Israr J, Li M (2017) Inception of geohydraulic failures in granular soils –
649 an experimental and theoretical treatment. *Géotechnique* 68:233–248.
650 <https://doi.org/10.1680/jgeot.16.P.227>
- 651 8. Cundall PA, Strack ODL (1979) A discrete numerical model for granular assemblies.
652 *Géotechnique* 29:47–65. <https://doi.org/10.1680/geot.1979.29.1.47>
- 653 9. O’Sullivan C (2011) *Particulate Discrete Element Modelling - A Geomechanics*
654 *Perspective*. London: Spon Press/Taylor & Francis

- 655 10. Barreto D (2009) Numerical and experimental investigation into the behaviour of
656 granular materials under generalised stress states. PhD. Thesis, University of London
- 657 11. Thornton C (2000) Numerical simulations of deviatoric shear deformation of granular
658 media. *Geotechnique* 50:43–53
- 659 12. Fonseca J, O’Sullivan C, Coop MR, Lee PD (2013) Quantifying the evolution of soil
660 fabric during shearing using directional parameters. *Geotechnique* 63:487–499.
661 <https://doi.org/http://dx.doi.org/10.1680/geot.12.P.003>
- 662 13. Fonseca J, O’Sullivan C, Coop MR, Lee PD (2013) Quantifying the evolution of soil
663 fabric during shearing using scalar parameters. *Geotechnique* 63:818–829.
664 <https://doi.org/10.1680/geot.11.P.150>
- 665 14. Cundall PA, Strack ODL (1983) Modeling of microscopic mechanisms in granular
666 material. *Stud Appl Mech* 7:137–149. [https://doi.org/10.1016/B978-0-444-42192-](https://doi.org/10.1016/B978-0-444-42192-0.50018-9)
667 [0.50018-9](https://doi.org/10.1016/B978-0-444-42192-0.50018-9)
- 668 15. Nguyen TT, Indraratna B (2020) The energy transformation of internal erosion based
669 on fluid-particle coupling. *Comput Geotech* 121:103475.
670 <https://doi.org/10.1016/j.compgeo.2020.103475>
- 671 16. Nguyen TT, Indraratna B (2020) A Coupled CFD–DEM Approach to Examine the
672 Hydraulic Critical State of Soil under Increasing Hydraulic Gradient. *ASCE Int J*
673 *Geomech* 20:04020138. [https://doi.org/10.1061/\(ASCE\)gm.1943-5622.0001782](https://doi.org/10.1061/(ASCE)gm.1943-5622.0001782)
- 674 17. Wautier A, Bonelli S, Nicot F (2018) Flow impact on granular force chains and
675 induced instability. *Phys Rev E* 98:42909.
676 <https://doi.org/10.1103/PhysRevE.98.042909>
- 677 18. Catalano E, Chareyre B, Barthélemy E (2014) Pore-scale modeling of fluid-particle
678 interaction and emerging poromechanical effects. *Int J Numer Anal Methods Geomech*
679 38:51–71

- 680 19. Galindo-Torres SA, Scheuermann A, Mühlhaus HB, Williams DJ (2015) A micro-
681 mechanical approach for the study of contact erosion. *Acta Geotech* 10:357–368.
682 <https://doi.org/10.1007/s11440-013-0282-z>
- 683 20. Han Y, Cundall P (2017) Verification of two-dimensional LBM-DEM coupling
684 approach and its application in modeling episodic sand production in borehole.
685 *Petroleum* 3:179–189. <https://doi.org/10.1016/j.petlm.2016.07.001>
- 686 21. Indraratna B, Phan NM, Nguyen TT, Huang J (2021) Simulating Subgrade Soil
687 Fluidization Using LBM-DEM Coupling. *ASCE Int J Geomech* 21:1–14.
688 [https://doi.org/10.1061/\(ASCE\)GM.1943-5622.0001997](https://doi.org/10.1061/(ASCE)GM.1943-5622.0001997)
- 689 22. Wu S, Chen Y, Zhu Y, et al (2021) Study on filtration process of geotextile with LBM-
690 DEM-DLVO coupling method. *Geotext Geomembranes* 49:166–179.
691 <https://doi.org/10.1016/j.geotexmem.2020.09.011>
- 692 23. Harshani HMD, Galindo-Torres SA, Scheuermann A, Mühlhaus HB (2015) Micro-
693 mechanical analysis on the onset of erosion in granular materials. *Philos Mag*
694 95:3146–3166. <https://doi.org/10.1080/14786435.2015.1049237>
- 695 24. Benseghier Z, Cuéllar P, Luu LH, et al (2020) A parallel GPU-based computational
696 framework for the micromechanical analysis of geotechnical and erosion problems.
697 *Comput. Geotech.* 120:103404
- 698 25. Ma Q, Wautier A, Zhou W (2021) Microscopic mechanism of particle detachment in
699 granular materials subjected to suffusion in anisotropic stress states. *Acta Geotech*
700 16:2575–2591. <https://doi.org/10.1007/s11440-021-01301-x>
- 701 26. Han K, Feng YT, Owen DRJ (2007) Numerical simulations of irregular particle
702 transport in turbulent flows using coupled LBM-DEM. *C - Comput Model Eng Sci*
703 18:87–100
- 704 27. Rettinger C, Råde U (2017) A comparative study of fluid-particle coupling methods

- 705 for fully resolved lattice Boltzmann simulations. *Comput Fluids* 154:74–89.
706 <https://doi.org/10.1016/j.compfluid.2017.05.033>
- 707 28. Seil P, Pirker S, Lichtenegger T (2018) Onset of sediment transport in mono- and
708 bidisperse beds under turbulent shear flow. *Comput Part Mech* 5:203–212.
709 <https://doi.org/10.1007/s40571-017-0163-6>
- 710 29. Chen S, Martínez D, Mei R (1996) On boundary conditions in lattice Boltzmann
711 methods. *Phys Fluids* 8:2527–2536. <https://doi.org/10.1063/1.869035>
- 712 30. Bhatnagar PL, Gross EP, Krook M (1954) A Model for Collision Processes in Gases .I.
713 Small Amplitude Processes in Charged and Neutral One-Component Systems. *Phys*
714 *Rev* 94:511–525. <https://doi.org/10.1103/PhysRev.94.511>
- 715 31. Noble DR, Torczynski JR (1998) A Lattice-Boltzmann Method for Partially Saturated
716 Computational Cells. *Int J Mod Phys C* 09:1189–1201.
717 <https://doi.org/10.1142/S0129183198001084>
- 718 32. Seil P (2016) LBDEMcoupling: Implementation, Validation, and Applications of a
719 Coupled Open-Source Solver for Fluid-Particle Systems. PhD. Thesis, JKU Johannes
720 Kepler Universität Linz
- 721 33. Kloss C, Goniva C, Hager A, et al (2012) Models, algorithms and validation for
722 opensource DEM and CFD-DEM. *Prog Comput Fluid Dyn An Int J* 12:140.
723 <https://doi.org/10.1504/PCFD.2012.047457>
- 724 34. Indraratna B, Haq S, Rujikiatkamjorn C, Israr J (2021) Microscale boundaries of
725 internally stable and unstable soils. *Acta Geotech*. [https://doi.org/10.1007/s11440-021-](https://doi.org/10.1007/s11440-021-01321-7)
726 [01321-7](https://doi.org/10.1007/s11440-021-01321-7)
- 727 35. Thornton C, Yang F, Seville J (2015) A DEM investigation of transitional behaviour in
728 gas-fluidised beds. *Powder Technol* 270:128–134.
729 <https://doi.org/10.1016/j.powtec.2014.10.017>

- 730 36. Kawano K, Shire T, O’Sullivan C (2018) Coupled particle-fluid simulations of the
731 initiation of suffusion. *Soils Found* 58:972–985.
732 <https://doi.org/10.1016/j.sandf.2018.05.008>
- 733 37. Abbireddy COR, Clayton CRI (2010) Varying initial void ratios for DEM simulations.
734 *Geotechnique* 60:497–502. <https://doi.org/10.1680/geot.2010.60.6.497>
- 735 38. Cundall PA (1988) Computer Simulations of Dense Sphere Assemblies. *Stud Appl*
736 *Mech* 20:113–123. <https://doi.org/10.1016/B978-0-444-70523-5.50021-7>
- 737 39. Senetakis K, Coop MR, Todisco MC (2013) Tangential load-deflection behaviour at
738 the contacts of soil particles. *Geotech Lett* 3:59–66.
739 <https://doi.org/10.1680/geolett.13.00019>
- 740 40. Hu Z, Zhang Y, Yang Z (2019) Suffusion-induced deformation and microstructural
741 change of granular soils: a coupled CFD–DEM study. *Acta Geotech* 14:795–814.
742 <https://doi.org/10.1007/s11440-019-00789-8>
- 743 41. Indraratna B, Israr J, Rujikiatkamjorn C (2015) Geometrical Method for Evaluating the
744 Internal Instability of Granular Filters Based on Constriction Size Distribution. *J*
745 *Geotech Geoenvironmental Eng* 141:04015045.
746 [https://doi.org/10.1061/\(ASCE\)GT.1943-5606.0001343](https://doi.org/10.1061/(ASCE)GT.1943-5606.0001343)
- 747 42. Huang X, Hanley KJ, O’Sullivan C, Kwok FCY (2014) Effect of sample size on the
748 response of DEM samples with a realistic grading. *Particuology* 15:107–115.
749 <https://doi.org/10.1016/j.partic.2013.07.006>
- 750 43. Jiang MJ, Konrad JM, Leroueil S (2003) An efficient technique for generating
751 homogeneous specimens for DEM studies. *Comput Geotech* 30:579–597.
752 [https://doi.org/10.1016/S0266-352X\(03\)00064-8](https://doi.org/10.1016/S0266-352X(03)00064-8)
- 753 44. Sufian A, Artigaut M, Shire T, O’Sullivan C (2021) Influence of Fabric on Stress
754 Distribution in Gap-Graded Soil. *J Geotech Geoenvironmental Eng* 147:04021016.

- 755 [https://doi.org/10.1061/\(ASCE\)GT.1943-5606.0002487](https://doi.org/10.1061/(ASCE)GT.1943-5606.0002487)
- 756 45. Ergun S (1952) Fluid Flow through Randomly Packed beds. *Chem Eng Prog* 48:89–94
- 757 46. Potyondy DO, Cundall PA (2004) A bonded-particle model for rock. *Int J Rock Mech*
758 *Min Sci* 41:1329–1364. <https://doi.org/10.1016/j.ijrmms.2004.09.011>
- 759 47. Li M, Fannin RJ (2012) A theoretical envelope for internal instability of cohesionless
760 soil. *Géotechnique* 62:77–80. <https://doi.org/10.1680/geot.10.T.019>
- 761 48. Imole OI, Kumar N, Magnanimo V, Luding S (2012) Hydrostatic and shear behavior
762 of frictionless granular assemblies under different deformation conditions. *KONA*
763 *Powder Part J* 30:84–108. <https://doi.org/10.14356/kona.2013011>
- 764 49. Thornton C, Antony SJ (1998) Quasi-static deformation of particulate media. *Philos*
765 *Trans R Soc A Math Phys Eng Sci* 356:2763–2782.
766 <https://doi.org/10.1098/rsta.1998.0296>
- 767 50. Cundall PA, Drescher A, Strack ODL (1982) Numerical experiments on granular
768 assemblies; measurements and observations. *Deform Fail Granul Mater IUTAM Symp*
769 *Delft* 355–370
- 770 51. Han K, Feng YT, Owen DRJ (2007) Coupled lattice Boltzmann and discrete element
771 modelling of fluid-particle interaction problems. *Comput Struct* 85:1080–1088.
772 <https://doi.org/10.1016/j.compstruc.2006.11.016>
- 773 52. Latt J (2008) Choice of units in lattice Boltzmann simulations. 1–6
- 774 53. Ten Cate A, Nieuwstad CH, Derksen JJ, Van den Akker HEA (2002) Particle imaging
775 velocimetry experiments and lattice-Boltzmann simulations on a single sphere settling
776 under gravity. *Phys Fluids* 14:4012–4025. <https://doi.org/10.1063/1.1512918>
- 777 54. Mindlin RD, Deresiewicz H (1989) Elastic Spheres in Contact Under Varying Oblique
778 Forces. In: *The Collected Papers of Raymond D. Mindlin Volume I*. pp 269–286
- 779 55. Tsuji Y, Tanaka T, Ishida T (1992) Lagrangian numerical simulation of plug flow of

780 cohesionless particles in a horizontal pipe. *Powder Technol* 71:239–250.

781 [https://doi.org/10.1016/0032-5910\(92\)88030-L](https://doi.org/10.1016/0032-5910(92)88030-L)

782

783 **LIST OF TABLES**

784 **Table 1.** Fluid properties for simulating the single-particle falling into the fluid using the
785 LBM-DEM approach (after Ten Cate et al. [53]).

786 **LIST OF FIGURES**

787 **Fig. 1.** Flowchart of the Lattice Boltzmann Method (LBM) combined with the Discrete
788 Element Method (DEM).

789 **Fig. 2.** (a) Particle size distribution of the sample selected for modelling in DEM; (b) three-
790 dimensional sample modelled in DEM; (c) division of the sample into different layers with
791 the mentioned layer numbers and initial void ratios (e_{oi}); (d) a close-up view of the particles
792 modelled in the fluid mesh using the LBM-DEM approach.

793 **Fig. 3.** Calibration of the soil specimen fluidisation model by comparing the flow curves
794 obtained from the LBM-DEM and the documented experimental work.

795 **Fig. 4.** (a) Evolution of overall hydraulic gradient with time; (b) Evolution of the increasing
796 local hydraulic gradient (i_{hyd}) and the decreasing normalised effective stresses ($\sigma'_{zz}/\sigma'_{zz0}$) (For
797 each layer, the eight symbols correspond to the initial state and the seven increase in the
798 overall hydraulic gradient (Fig 4(a)))

799 **Fig. 5.** (a) Division of the sample into different layers with the indicated layer numbers and
800 coefficient of earth pressure (K) values at the hydrostatic state, (b) Development of the
801 normalised horizontal and vertical effective stress with hydraulic gradient

802 **Fig. 6.** Evolution of increasing broken contacts (B_R) with the decreasing normalised effective
803 stresses ($\sigma'_{zz}/\sigma'_{zz0}$) (For each layer, the eight symbols correspond to the initial state and the
804 seven increase in the overall hydraulic gradient (Fig 4(a)))

805 **Fig. 7.** Development of the decreasing fraction of mechanically stable particles (M_s) with
806 decreasing normalised effective stresses ($\sigma'_{zz}/\sigma'_{zz0}$) (For each layer, the eight symbols
807 correspond to the initial state and the seven increase in the overall hydraulic gradient (Fig
808 4(a)))

809 **Fig. 8.** Conceptual model showing the differences in the fabrics of particles with the same
810 void ratios.

811 **Fig. 9.** Cumulative distributions of the coordination number (Z) at the hydrostatic state and
812 the onset of fluidisation of soil specimen.

813 **Fig. 10.** Development of the decreasing average coordination number (Z_{avg}) with decreasing
814 normalised effective stresses ($\sigma'_{zz}/\sigma'_{zz0}$) (For each layer, the eight symbols correspond to the
815 initial state and the seven increase in the overall hydraulic gradient (Fig 4(a)))

816 **Fig. 11.** Distribution of the sliding index (S_i) of the selected Layer 10 with different local
817 hydraulic gradients (i_{hyd}).

818 **Fig. 12.** (a) Three-dimensional representation of the hydraulic gradient (i_{hyd}), the normalised
819 effective stresses ($\sigma'_{zz}/\sigma'_{zz0}$), and the constraint ratio (R); (b) projections of the three-
820 dimensional plot of i_{hyd} , $\sigma'_{zz}/\sigma'_{zz0}$, and R (For each layer, the eight symbols correspond to the
821 initial state and the seven increase in the overall hydraulic gradient (Fig 4(a)))

822 **Fig. A.1.** Directions of the 19 (0-18) velocity vectors of the $D3Q19$ discretisation scheme
823 used in this study.

824 **Fig. A.2.** (a) Schematic representation of a single sphere falling into the fluid with a diameter
825 (d_p) = 15 mm; (b) the modelled particle in the fluid mesh using LBM-DEM; (c) comparison
826 of the numerical and experimental results of particle position over time; (d) comparison of
827 experimental and numerical results of particle velocity over time.

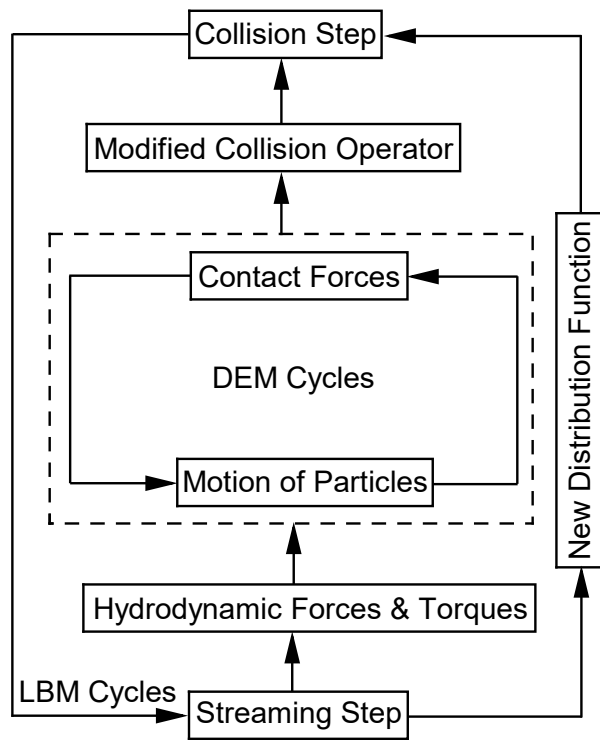
828 **Fig. B.1.** (a) Rheological scheme and (b) schematic sketch of the Hertz-Mindlin contact
829 model used in this study to simulate fluidisation of soil specimen.

830 **Table 1.** Fluid properties for simulating the single-particle falling into the fluid using the

831 LBM-DEM approach (after Ten Cate et al. [53]).

832

Case	Density (ρ_f) (kg/m³)	Kinematic Viscosity (ν_f) (m²/s)
$Re_p = 1.5$	970	3.845×10^{-4}
$Re_p = 4.1$	965	2.197×10^{-4}
$Re_p = 11.6$	962	1.175×10^{-4}
$Re_p = 31.9$	960	6.042×10^{-5}



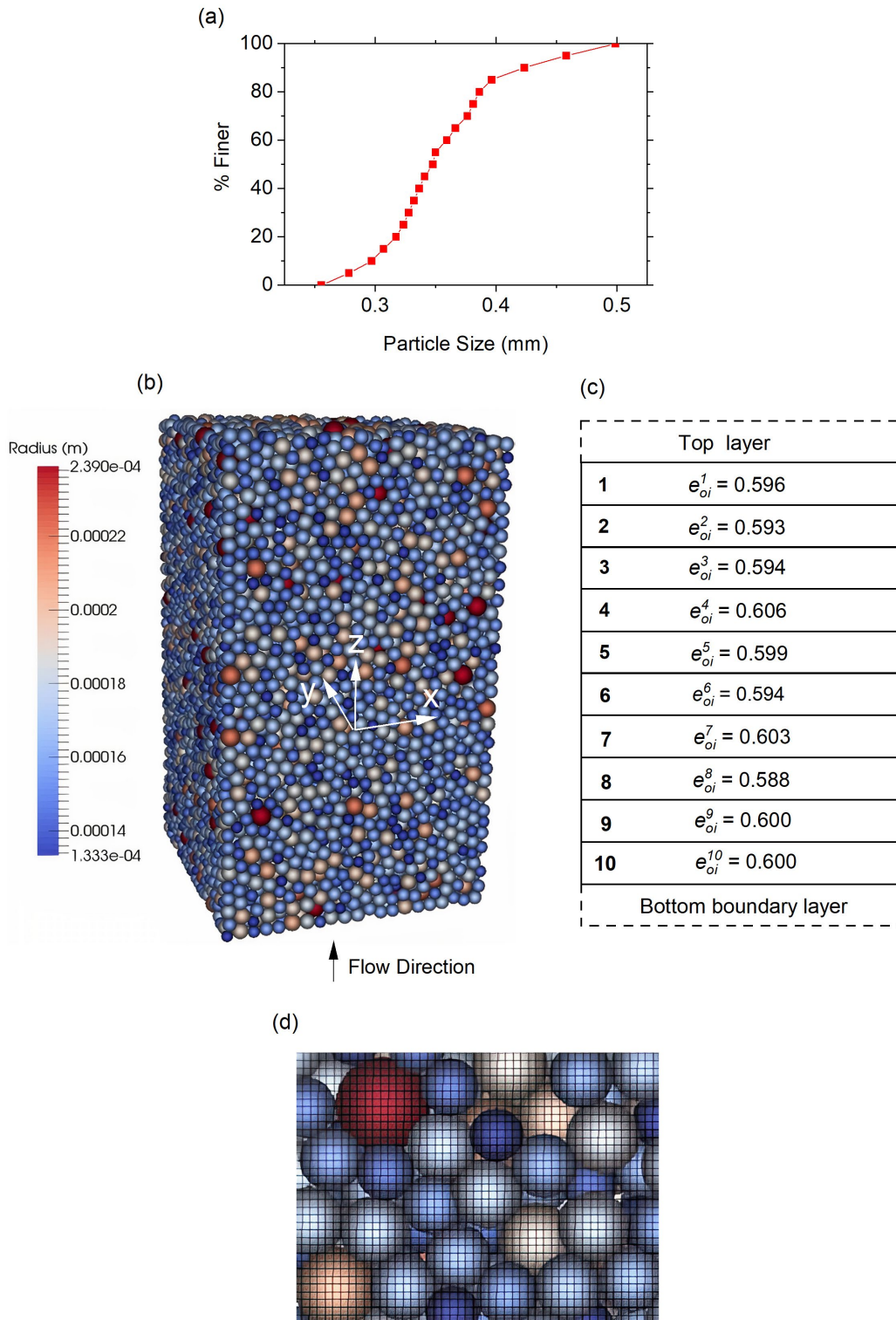
833

834

Fig. 1. Flowchart of the Lattice Boltzmann Method (LBM) combined with the Discrete

835

Element Method (DEM)



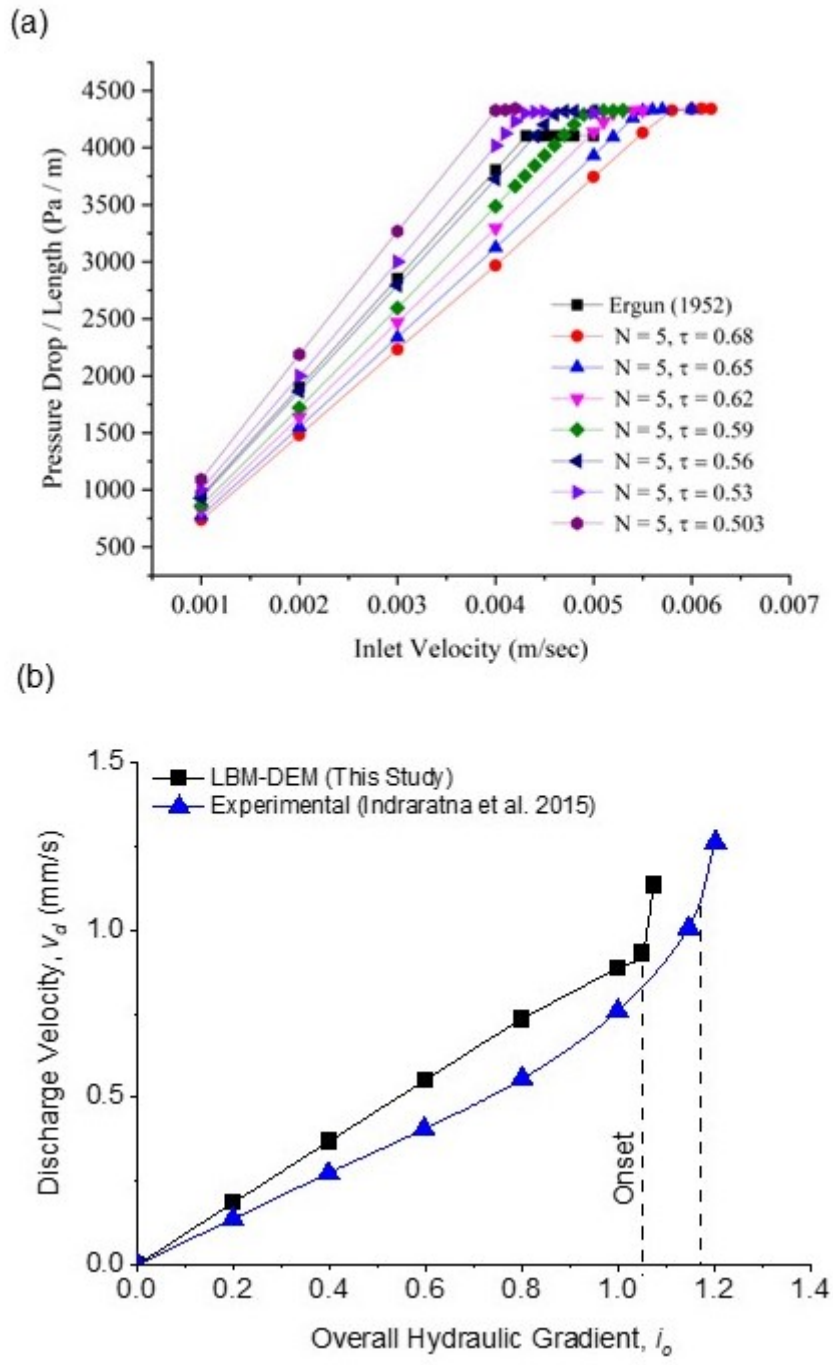
836

837 **Fig. 2.** (a) Particle size distribution of the sample selected for modelling in DEM; (b) three-

838 dimensional sample modelled in DEM; (c) division of the sample into different layers with

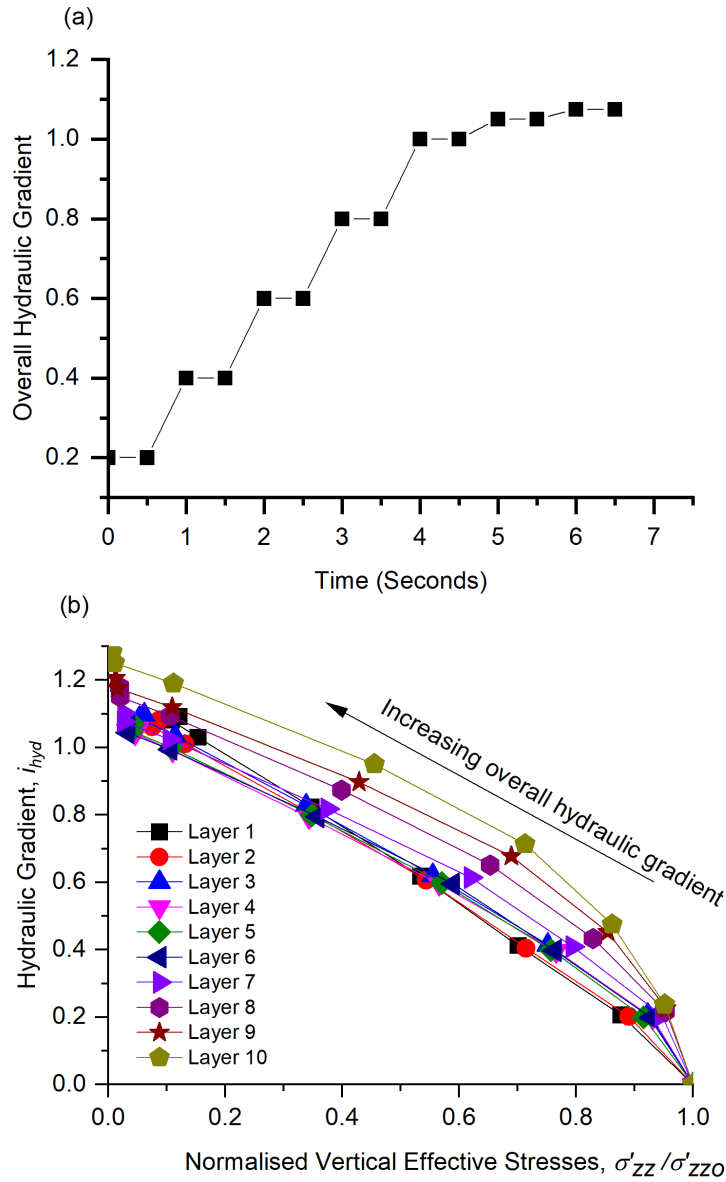
839 the mentioned layer numbers and initial void ratios (e_{oi}); (d) a close-up view of the particles

840 modelled in the fluid mesh using the LBM-DEM approach



841

842 **Fig. 3.** (a) Calibration of the relaxation parameter by comparing the pressure drops obtained
 843 from the LBM-DEM and an analytical solution, (b) Comparison of the flow curves obtained
 844 from the LBM-DEM and the documented experimental work



845

846 **Fig. 4.** (a) Evolution of overall hydraulic gradient over time; (b) Evolution of the increasing

847 local hydraulic gradient (i_{hyd}) and the decreasing normalised vertical effective stresses

848 ($\sigma'_{zz}/\sigma'_{zZo}$) (For each layer, the eight symbols correspond to the initial state and the seven

849 increase in the overall hydraulic gradient (Fig 4(a)))

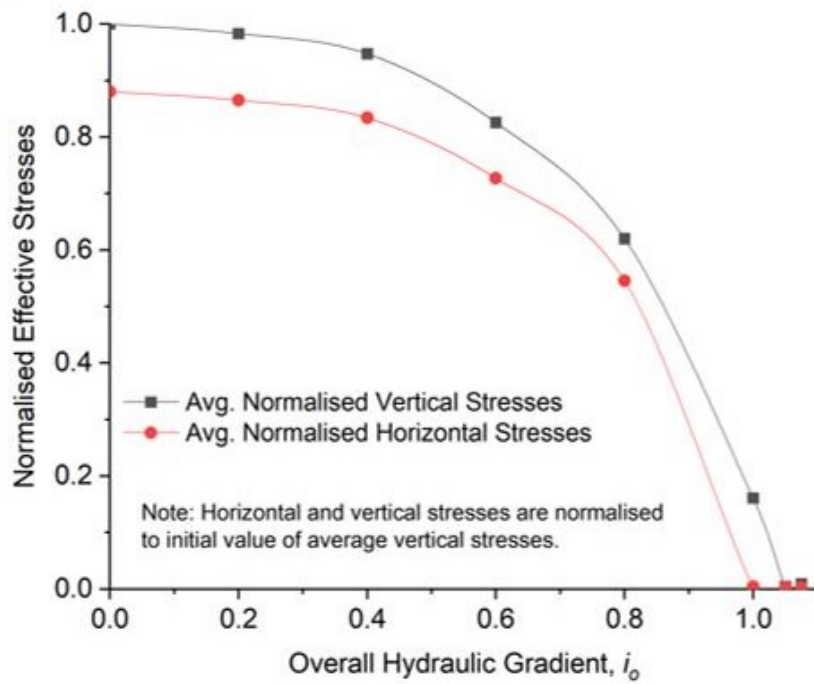
850

851

(a)

Top layer	
1	$K^1 = 0.90$
2	$K^2 = 0.89$
3	$K^3 = 0.89$
4	$K_o^4 = 0.88$
5	$K^5 = 0.88$
6	$K^6 = 0.87$
7	$K^7 = 0.87$
8	$K^8 = 0.87$
9	$K^9 = 0.86$
10	$K^{10} = 0.86$
Bottom boundary layer	

(b)



852

853

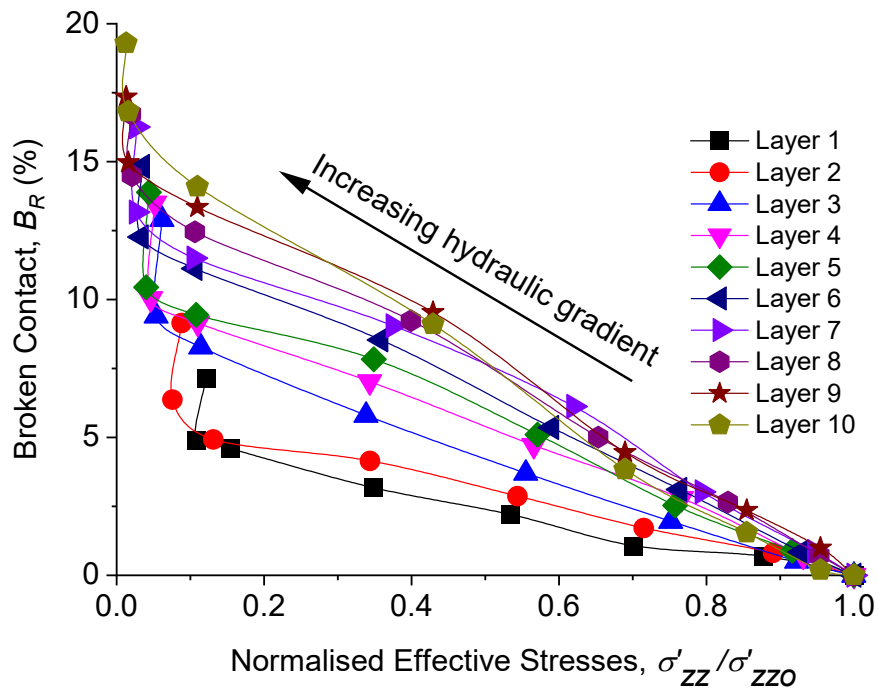
Fig. 5. (a) Division of the sample into different layers with the indicated layer numbers and

854

coefficient of earth pressure (K) values at the hydrostatic state, (b) Development of the

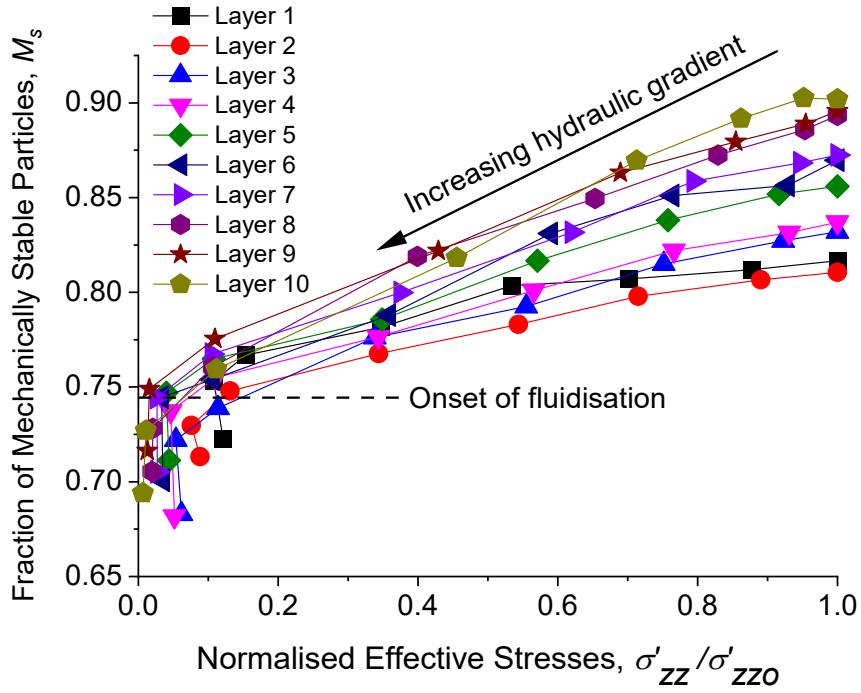
855

normalised horizontal and vertical effective stress with hydraulic gradient



856

857 **Fig. 6.** Evolution of increasing broken contacts (B_R) with the decreasing normalised effective
 858 stresses ($\sigma'_{zz}/\sigma'_{zz0}$) (For each layer, the eight symbols correspond to the initial state and the
 859 seven increase in the overall hydraulic gradient (Fig 4(a)))



860

861

Fig. 7. Development of the decreasing fraction of mechanically stable particles (M_s) with

862

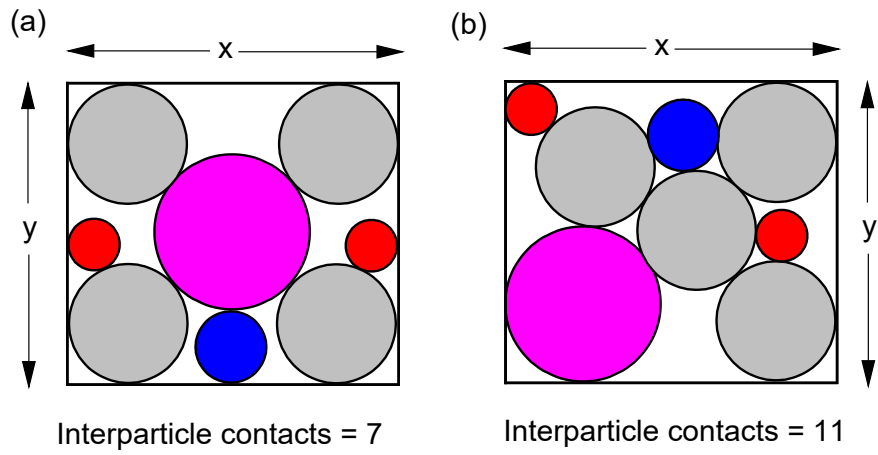
decreasing normalised effective stresses ($\sigma'_{zz}/\sigma'_{zzo}$) (For each layer, the eight symbols

863

correspond to the initial state and the seven increase in the overall hydraulic gradient (Fig

864

4(a))

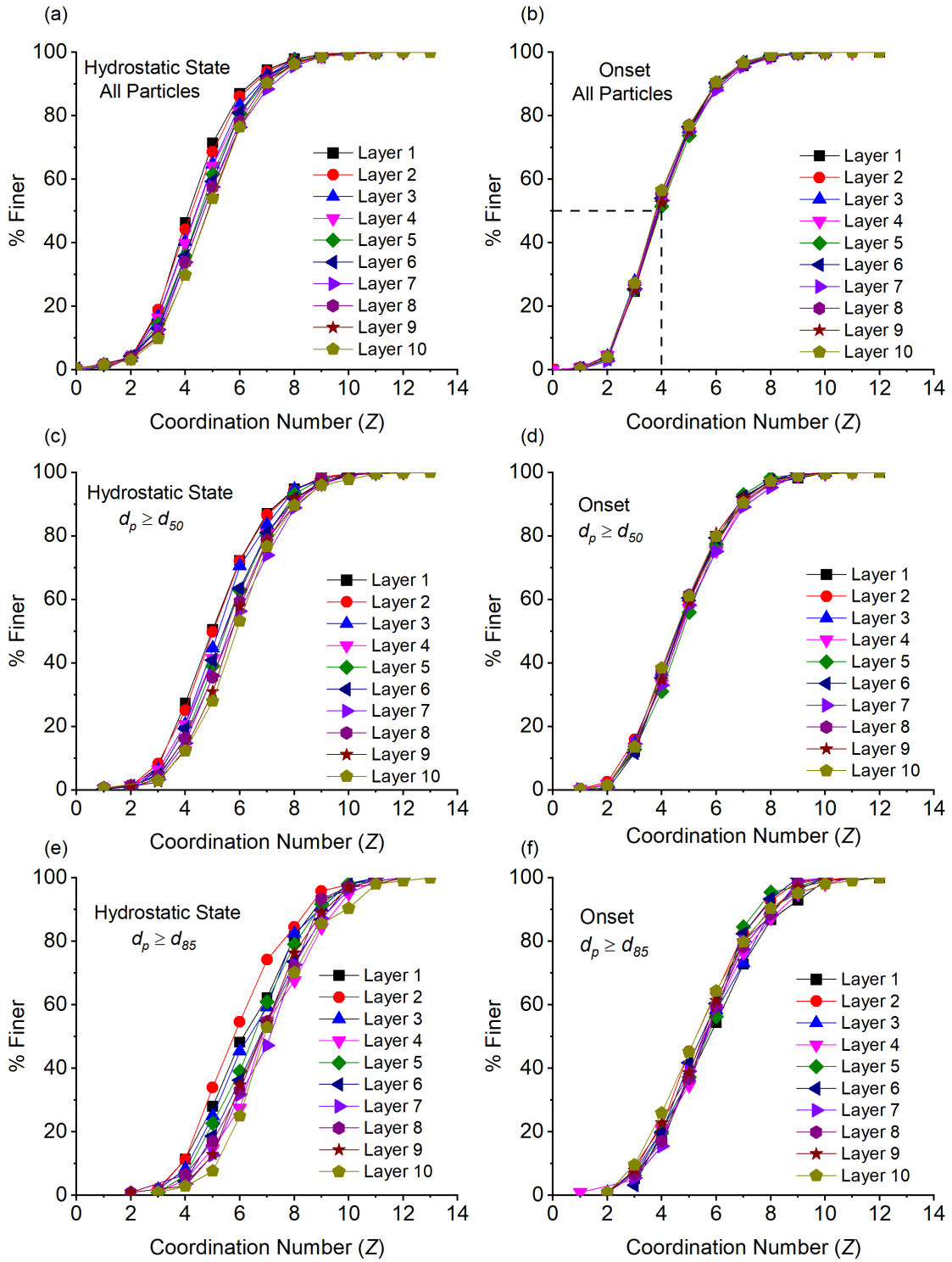


865

866 **Fig. 8.** Conceptual model showing the differences in the fabrics of particles with the same

867

void ratios

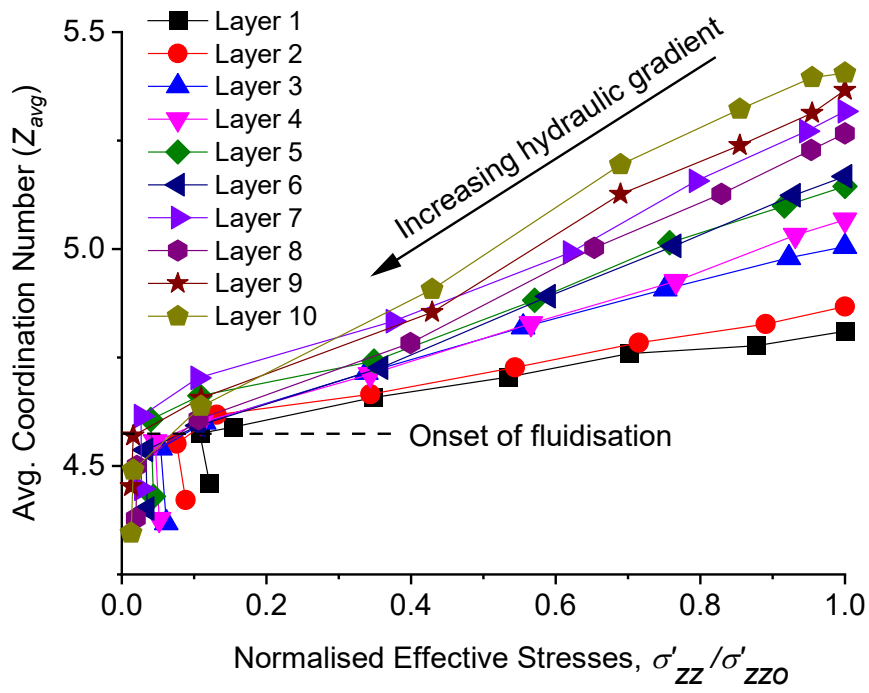


868

869 **Fig. 9.** Cumulative distributions of the coordination number (Z) at the hydrostatic state and

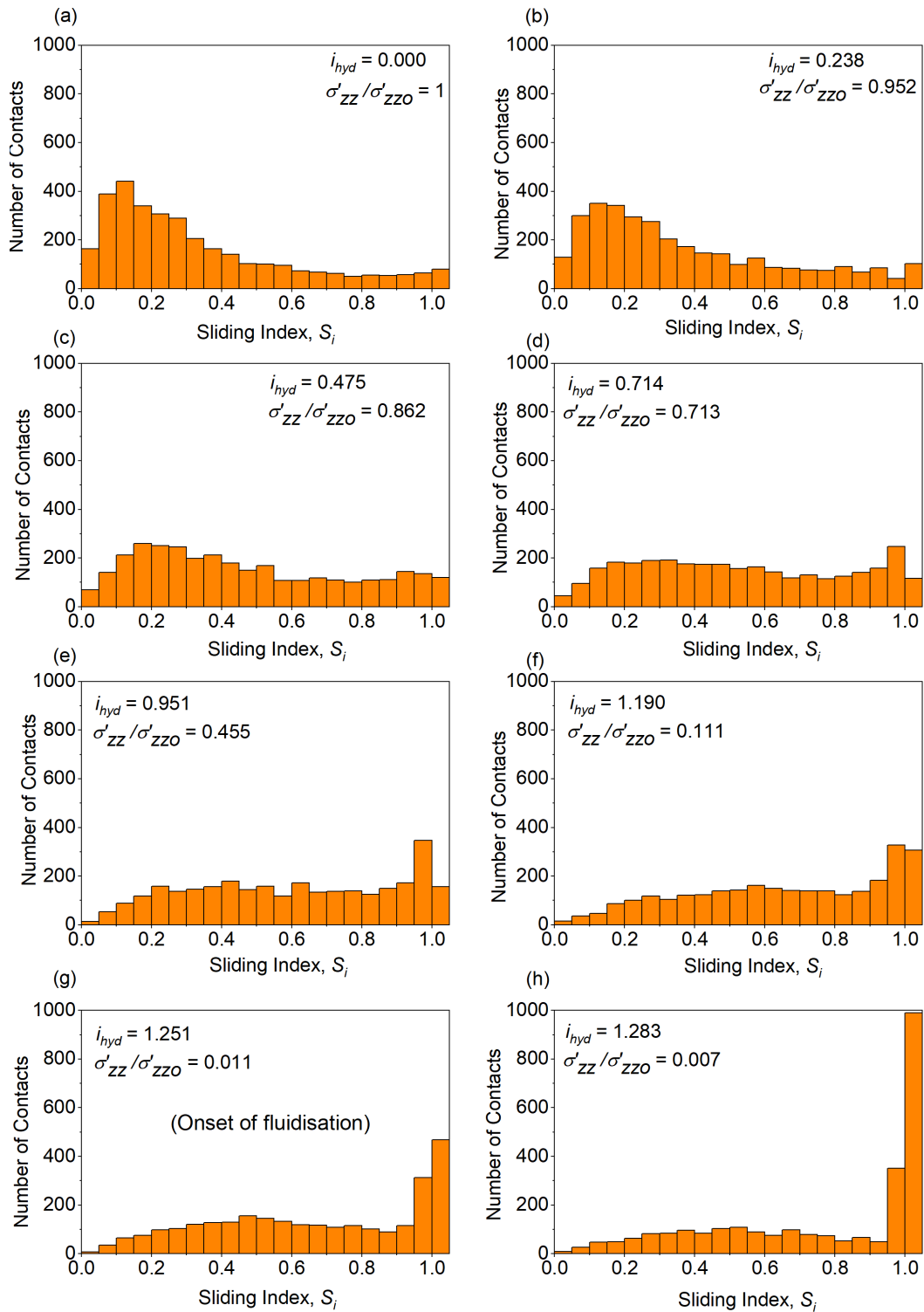
870

the onset of fluidisation of soil specimen



871

872 **Fig. 10.** Development of the decreasing average coordination number (Z_{avg}) with decreasing
 873 normalised effective stresses ($\sigma'_{zz}/\sigma'_{zz0}$) (For each layer, the eight symbols correspond to the
 874 initial state and the seven increase in the overall hydraulic gradient (Fig 4(a)))

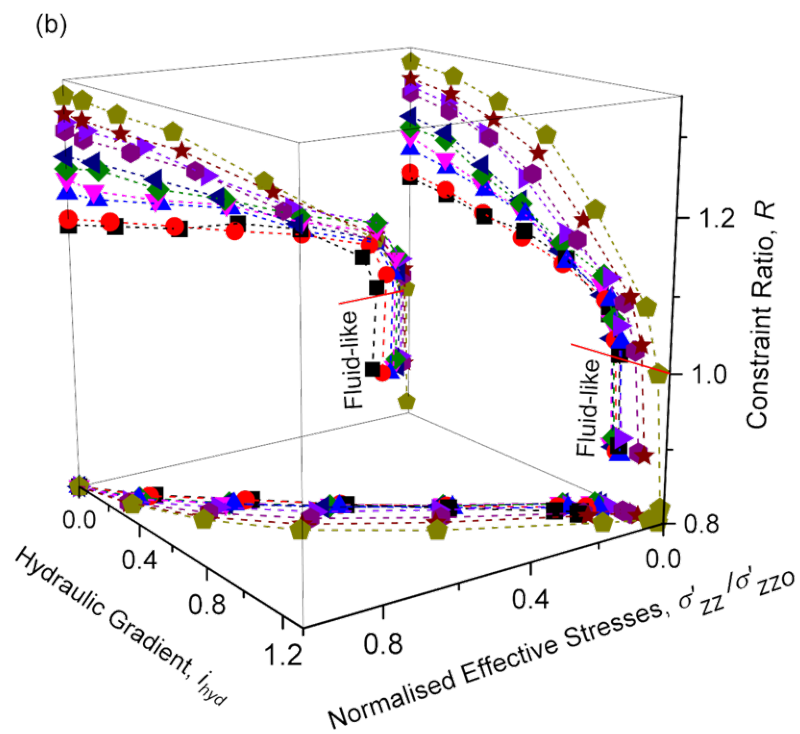
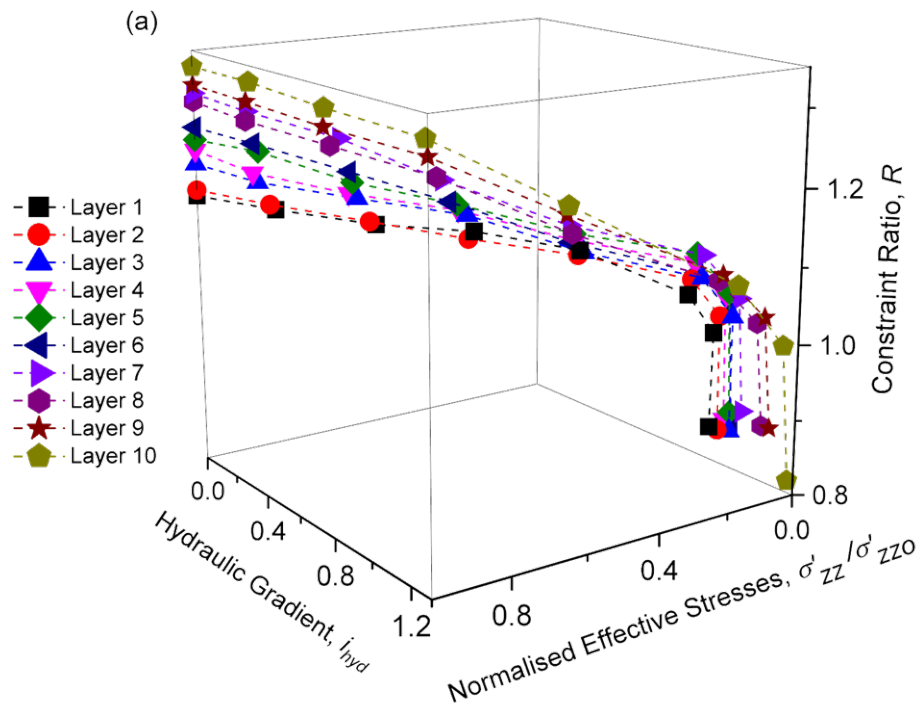


875

876

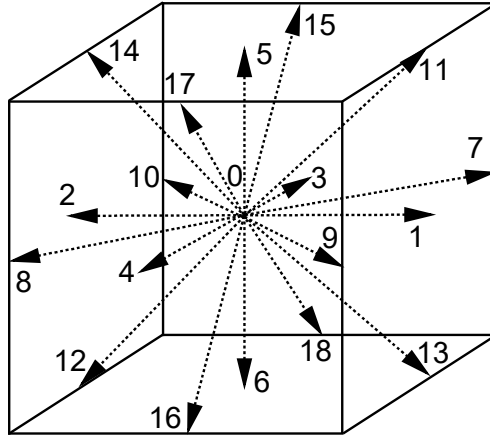
Fig. 11. Distribution of the sliding index (S_i) of the selected Layer 10 with different local hydraulic gradients (i_{hyd})

877



878

879 **Fig. 12.** (a) Three-dimensional representation of the hydraulic gradient (i_{hyd}), the normalised
 880 effective stresses ($\sigma'_{zz}/\sigma'_{zZo}$), and the constraint ratio (R); (b) projections of the three-
 881 dimensional plot of i_{hyd} , $\sigma'_{zz}/\sigma'_{zZo}$, and R (For each layer, the eight symbols correspond to the
 882 initial state and the seven increase in the overall hydraulic gradient (Fig 4(a)))



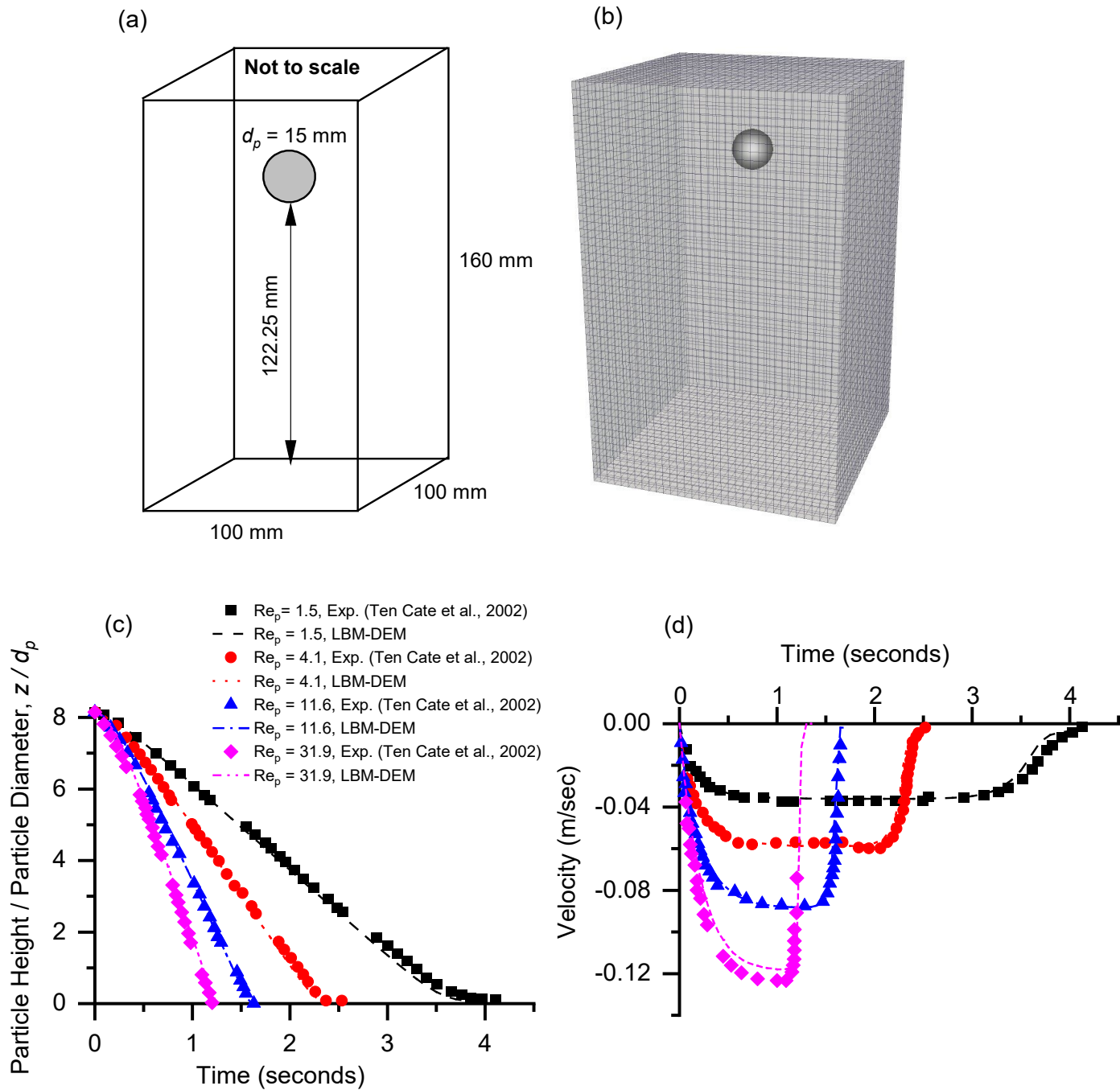
883

884 **Fig. A.1.** Directions of the 19 (0-18) velocity vectors of the $D3Q19$ discretisation scheme

885

used in this study

886



887

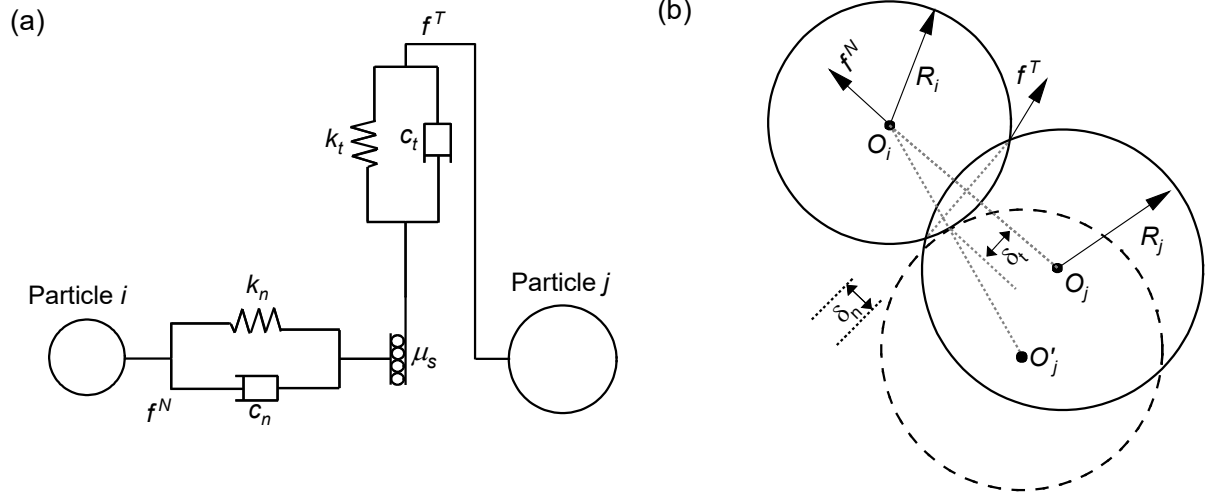
888 **Fig. A.2.** (a) Schematic representation of a single sphere falling into the fluid with a diameter

889 (d_p) = 15 mm; (b) the modelled particle in the fluid mesh using LBM-DEM; (c) comparison

890 of the numerical and experimental results of particle position over time; (d) comparison of

891 experimental and numerical results of particle velocity over time.

892



893

894 **Fig. B.1.** (a) Rheological scheme and (b) schematic sketch of the Hertz-Mindlin contact

895 model used in this study to simulate the fluidisation of a soil specimen.