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 Particle-Scale Observation of Seepage Flow in Granular Soils Using PIV and CFD
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7

# 8 Abstract

9 Seepage-induced instabilities pose a challenge in many geotechnical applications. Particle-scale 10 mechanisms govern the initiation of instability. However, current understanding is based on a 11 macro-scale perspective that draws on continuum mechanics. Recent developments in imaging and 12 numerical analysis can provide the particle-scale fundamental perspective needed to develop a 13 comprehensive insight. This contribution demonstrates the value of combining particle-scale experimental and numerical studies. The experiments consider transparent soil samples created 14 15 using refractive image matching and monitored by particle image velocimetry (PIV). Three-16 dimensional pore topology is extracted from a series of 2D images and imported into computational fluid dynamics (CFD) simulations. Permeability is estimated by three distinct 17 approaches: using flow rate, PIV- and CFD-generated data. The flow fields obtained from PIV and 18 19 CFD are in good agreement considering both flow rate contour plots and flow rate distributions; this demonstrates the successful reconstruction of three-dimensional pore structure and flow-field 20 21 analysis. The comparison also reveals that the side boundary effects in CFD simulations are 22 constrained within a limited region. The multi-plane results characterize the variance of flow

23	velocity with the three-dimensional pore topology. Finally, the fluid-particle interactions obtained
24	from CFD results show a larger variance in the angular particle packings.
25	
26	Keywords: Particle-scale behaviour; permeability; seepage; laboratory tests; numerical modelling
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30 1. Introduction
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A comprehensive understanding of seepage flow in cohesionless or granular soils is critical in 31 32 many geotechnical analyses associated with dewatering, dam and flood embankment design, slope 33 stability etc. Seepage analyses to inform engineering design typically adopt a continuum approach with macro-scale parameters. However, the fundamental processes that lead to the internal erosion 34 35 in embankment dams (ICOLD, 2015) and settlement due to fines migration during dewatering 36 (Preene & Rosser, 2012) initiate at the particle scale. Understanding these processes is important 37 to inform robust approaches to design, e.g. considering whether to continue to use hydraulic 38 gradient rather than seepage velocity when assessing the risk of a seepage-induced instability 39 (Vogt et al., 2015). Incidents such as the failure of Gouhou Dam in 1993 (Zhang & Chen, 2006) 40 and the serious sinkhole incident at WAC Bennett dam in Canada in 1996 (Muir Wood, 2007) 41 remind us of the significant hazard that can be posed by seepage instabilities. Globally, seepage 42 instabilities have caused about 50% of recorded embankment dam failures (Foster et al., 2000). 43 This contribution adopts a combination of particle image velocimetry (PIV) and computational 44 fluid dynamics (CFD) to quantify seepage flow in the void space of a transparent granular soil and 45 to determine the fluid-particle interaction forces that can lead to particle migration and instability.

46 Saturated transparent soils can be created by refractive index (RI) matching between model (analogue) sands formed of borosilicate glass and carefully selected pore fluids. Illumination by a 47 laser light sheet enables visualization of the particles along a plane within the material, and so the 48 49 internal mechanisms that underlie complex macro-scale behaviours can be studied (Hunter & Bowman, 2018; Iskander et al., 2015). Hunter and Bowman (2018) developed a transparent soil 50 51 rigid-walled permeameter to study the particle-scale mechanisms that occur during internal erosion 52 in gap graded particulate systems. They considered a single plane within the sample and successfully imaged particle migration. However, there was no local measurement of fluid flow, 53 54 and the data generated were two-dimensional. Saleh et al. (1992) and Northrup et al. (1993) applied 55 Particle Imaging Velocimetry (PIV) to tracer particles in the pore fluid to generate 2D images of flow in transparent porous media created using RI matching. Peurrung et al. (1995) applied Particle 56 57 Tracking Velocimetry using a similar experimental set-up, again obtaining 2D data. Alternatively, 58 the flow fields in 2D transparent micromodels fabricated with soft lithography may be determined with micro-PIV (Karadimitriou et al., 2013; Karadimitriou & Hassanizadeh, 2012; Meinhart et al., 59 60 1999). However, it is the 3D geometry of the void space that controls flow in the pores; a complete picture cannot be obtained from planar data. 3D flow data can be obtained using tomographic 61 62 technologies which can be used on opaque materials, e.g. Magnetic Resonance Imaging MRI and Particle Emission Tomography PET (Khalili et al., 1998; Sederman et al., 1997). However, the 63 data generated are often of limited spatial or temporal resolution. 64

Computational fluid dynamics (CFD) has been applied to study flow in porous rocks
(Mostaghimi et al., 2013; Nunes et al., 2015; Piller et al., 2014) and in sands (Garcia et al., 2009;
Taylor et al., 2016, 2017). In these studies, the topology of the pore space was obtained from
micro-computed tomography scans. The volumes of soil/rock considered was relatively small, and

69 ideal flow boundary conditions were typically assumed along the sides of the sample. While the 70 resulting permeabilities appeared reasonable, the accuracy of the velocities within the pores could 71 not be verified, and the implications of the idealized boundary conditions could not be quantified. 72 Huang et al. (2008) and Thaker et al. (2019) determined the 3D topology of the void space in 73 transparent samples, and applied CFD to simulate flow and compared these data with flow field 74 data acquired using PIV. However, the comparisons considered only a single plane and spherical 75 particles.

Developing the work of Hunter & Bowman (2018), this study adopts refractive-index-matched 76 77 transparent materials and PIV to monitor the flow field in a transparent permeameter. A method 78 was developed to precisely control the laser sheet position in order to enable multiple images of 79 the pore topology and the fluid-flow field to be acquired so that, in contrast to earlier studies, quasi-80 3D experimental data were recorded. Three-dimensional pore topologies reconstructed from sliceby-slice scanning and image processing are incorporated in CFD simulations. This combination of 81 laboratory experiments and numerical modelling enables the following questions to be addressed: 82 83 i) Can PIV be used to develop a three-dimensional understanding of seepage flow in the void space of granular soils? 84

# 85 ii) To what extent do the assumed flow boundary conditions compromise the accuracy of the 86 predictions of the local fluid velocities in CFD analyses of seepage flow in the void space 87 of soil?

88 iii) Particle migration induced by the fluid-particle interaction force initiates all of the
89 instabilities noted above. Can the combined PIV and CFD analyses enable quantification
90 of the fluid-particle interaction forces in real physical systems?

In a preliminary application of the approach proposed here, we considered two materials with very
different particle morphologies and show how this technique can be used to explore the influence
of morphology on flow fields and fluid-particle interaction forces.

94

# 95 **2. Experimental Setup**

### 96 **2.1.** Transparent soil permeameter

The experimental apparatus is a rigid-walled 'transparent soil' permeameter that has been 97 designed to visualize the mechanisms occurring during seepage-induced internal erosion in 98 99 susceptible granular media (Hunter & Bowman, 2018). Fig.1 is a sketch of the experimental device. 100 The permeameter is a rectangular cell (100 mm by 100 mm in plan area and 265 mm high). Five 101 vertical manometer ports are arranged at the back of the permeameter for local head measurements. 102 The flow is directed upward via a constant head applied at the base using an adjustable header tank. 103 Flow from the top of the cell is recirculated back into a reservoir and then pumped back into the 104 header tank. A constant head was applied, and the resulting local head values were measured using the manometers located at the back of the permeameter cell. Consideration was restricted to 105 106 laminar, low Reynolds number flows, typically encountered in geotechnical applications. Particle 107 movement was not expected since the drag forces were relatively low compared with the particle 108 weights (i.e. gravitational force). Also, analysis of the images showed no visible particle movement 109 throughout testing.

### 110 **2.2.** Laser and imaging systems

A 1.5 mm thick laser sheet parallel to the direction of the flow was applied to the side of the 111 112 permeameter to illuminate a selected plane perpendicular to the z-axis in Figure 1. The light source was a 1W Kvant continuous wave laser at 520 nm (green) wavelength with variable power control. 113 114 The laser beam was coupled from the laser head into an optical fibre, recollimated at the fibre 115 output, and then sent through a line generator lens mounted on a lens post and base plate to provide height adjustment. This optical assembly was fixed on a linear micrometre stage with a 25 mm 116 travel range so that specific planes of interest could be imaged and returned to with precision over 117 long-running tests. 118

119 A high-speed camera, Phantom Miro 310, mounted on another linear micrometre stage with a 120 50 mm travel range was positioned in front of the permeameter cell to record images with a spatial 121 resolution of  $1280 \times 800$  pixels at 200 frames/s. During each test, the position of the camera in the 122 z-direction was adjusted in accordance with the laser sheet position to retain a sharp image focus. 123 A Nikon AF Nikkor lens 85 mm was used with up to 34 mm of extension rings placed between 124 the lens and the camera sensor. All images were recorded using an aperture *f*-stop number of 4, 125 which was selected according to its influence on the tracer magnification, as discussed later.

# 126 **2.3.** Tested materials

Table 1 shows the physical and optical properties of the two model soils. The first sample consisted of  $7.5 \pm 0.03$  mm diameter spherical beads made of borosilicate glass purchased from SiliBeads. The second sample consisted of angular particles made from Duran® glass with size ranging from 6.7 to 9.5 mm (Sanvitale & Bowman, 2012).

131 The particle size was chosen based on a trade-off between different aspects related to the 132 optical technique, practical considerations and standard guidelines. As general rule, the size of the particles must be large enough to ensure the tracers can flow easily through the pores without 133 134 blocking the channels. In addition, the procedure for Standard Test Method for Permeability of Granular Soils (ASTM D 2434-68, 2000) requires the maximum particle size of the specimen to 135 136 be 8 to 12 times smaller than the diameter of the permeameter. Furthermore, in previous experimental work (Sanvitale & Bowman, 2012) the same refractive index matched material was 137 used and it was observed that the presence of small particles produces a greater amount of scattered 138 139 light in the granular system owing to the slight differences in refractive indices at the grain-liquid 140 interfaces. It was found that better transparency even at the deepest illuminated sections, can be 141 obtained when large particles are used. Finally, the availability in the laboratory of a sample of 142 angular particles (that are not commercially available but hand-made, see Sanvitale & Bowman 143 2012) with gradations comparable to those of the beads was taken into account, in order to carry out tests with grains of different shape but compatible drainage behaviour. 144

Each sample was prepared using a 'slurry' placement method to avoid entrapment of air bubbles (Hunter & Bowman, 2018) to create a sample approximately 165 mm in height. In order to develop a uniform pressure and velocity conditions entering the sample, a 45 mm layer of 'dispersing' filter material, comprising a mixture of spherical borosilicate beads of 15 mm and 10 mm diameter, was placed at the bottom of the apparatus.

A hydrocarbon immersion fluid (Cargille Laboratories) was chosen to match the refractive index of the glass particles (Sanvitale & Bowman, 2012; Wiederseiner et al., 2011). As well as a close optical match, the fluid and solid mixture needed to behave similarly to soil and water in terms of buoyancy. The effective specific gravity of the particles compared with the fluid was 2.64 154 - which is typical of soil in water. In order to achieve the best refractive index match during testing, 155 different room temperatures were used, 23 °C for the beads and 26 °C for the angular particles. 156 Figure 2(a) shows a typical outcome of refractive index matching under normal lighting conditions. 157 A small amount of Nile Red fluorescent dye, added to the fluid phase, enabled the application of 158 Planar Laser-Induced Fluorescence (PLIF) based imaging on identifying the solid particles with 159 respect to the fluid phase. To characterize the pore topology, the saturated sample was illuminated 160 by the laser sheet whose wavelength matched the absorption peak of the fluorescent dye within 161 the fluid. The resulting fluorescence (where the dye emits light at a wavelength greater than that 162 of the excitation wavelength) was recorded by the high-speed camera through a long-pass filter placed over the lens to transmit only the fluorescence signal and discard the green laser light: the 163 164 particles show as dark on a bright fluid background.

165

# 166 **3.** Particle Image Velocimetry (PIV) Analyses

# 167 *3.1.* Calibration for image size and distortion

Before each test, the image size and distortion were calibrated with fixed grid dots at 1 mm ± 0.001 mm spacing inside the permeameter cell filled with the liquid phase at the locations of the 26 vertical planes imaged in the experiment. The distortion error due to the optical assembly was corrected according to the procedure discussed in Gollin et al. (2017). The coordinates of the dots were estimated with sub-pixel accuracy and associated with an undistorted grid and then interpolated using a built-in MATLAB function Scattered-Interpolant (Brevis et al., 2011). This approach adopts a linear interpolation based on Delaunay triangulation. The fluid flow field was imaged using reflective seed tracers dispersed in the liquid phase. These seeding particles should be neutrally buoyant and small enough to follow the flow accurately. Silver-coated hollow microspheres with a nominal size ranging between 5-30  $\mu$ m were used at a concentration of 35 mg/l. These had a density of 0.75 g/cm<sup>3</sup>, resulting in an effective specific gravity of 1.13 compared to the fluid, i.e. close to unity. To ensure that the inertia effects due to particle density were negligible so that the tracers would reliably follow the flow, the Stokes number was calculated as follows:

$$Stk_s = \frac{\rho_s d_s^2 u_y}{18\nu\rho D} \ll 1 \tag{Eq. 1}$$

where  $d_s$  and  $\rho_s$  are the seed diameter and density, respectively, D the bead diameter, v and  $\rho$  the 183 184 fluid kinematic viscosity and density, respectively, and  $u_y$  is the axial (y-direction) fluid velocity of the flow. For our set-up, the maximum Stokes number was calculated to be  $Stk_s = 2.59 \times 10^{-6}$ . 185 186 The movement of the tracers was recorded by removing the long-pass filter in front of the camera lens to allow the light reflected from their surfaces to be captured. Figure 2(b) and (c) show how 187 laser illumination enables internal visualization of a plane within both spherical bead and angular 188 189 particle samples with the tracers. Two videos, V1 and V2 in the supplementary material, show the 190 movement of tracers in both spherical bead and angular particle samples. Figure 2(d) shows the top view of the laser sheet illuminated plane with a finite thickness of around 1.5 mm. 191

### *3.3. Image acquisition for 3D volumes*

193 The flow fields inside two 3D volumes were examined within each sample. The lower volumes 194 were located between manometer ports P2 and P3 and denoted as sub-volumes Beads-L and Ang195 L for the spherical sample and angular samples, respectively (Figure 1). The upper volumes were 196 located between manometer ports P3 and P4 and denoted as sub-volumes Beads-U and Ang-U, 197 respectively. The dimensions of sub-volumes varied slightly with the position of the high-speed 198 camera, as shown in Table 2. In each sub-volume, the flow fields on 26 planes parallel to the flow 199 directions were measured. These planes were evenly spaced at 1 mm ±0.001mm, centred in the mid-section of the permeameter cell with at least 32 mm distance from the lateral sidewalls. The 200 201 choice of inter-plane spacing was made based on the laser sheet thickness of 1.5 mm. On each plane, a series of images were taken over 2 seconds at 200 frames/s, i.e. 400 images were taken 202 203 per plane.

# 204 **3.4.** PIV postprocessing

An open-source software, PIVlab (Thielicke & Stamhuis, 2014), was used for image 205 processing to determine the flow velocities. PIVlab gives an Eulerian description of the 206 investigated velocity field, estimating the displacement for groups of tracers by determining the 207 208 peak of the cross-correlation of many small interrogation areas. This software uses a multi-pass 209 cross-correlation algorithm coupled with a window deformation technique to obtain the velocity vectors (Thielicke, 2014). The 2-step correlation algorithm with decreasing window size (D<sub>I</sub>) was 210 211 used to evaluate the recorded images with a final size of  $32 \times 32$  pixels (approximately  $1 \times 1$  mm<sup>2</sup> 212 area), set to minimize the loss of in-plane particle pairs ensuring that the x and y displacements 213 were smaller than DI/4. The loss of particle pairs between corresponding interrogation windows due to out-of-plane motion was limited due to the fact that the z displacement of the tracer particles, 214 215 which can be assumed to be of the same magnitude as the tracer particle displacement in the xdirection, was less than a quarter of the light sheet thickness (Atkins, 2016; Keane & Adrian, 1993).
The overlap of the interrogation windows was 50% for all steps.

218 The velocity fields for each plane position were calculated by averaging over 2 s of recorded 219 images, and the 'instantaneous velocities' were estimated on two successive frames separated by a time steps  $\Delta t$ . The frame rate was 200 fps for all of the experiments. The influence of the time 220 step on the fluid velocities was studied by setting  $\Delta t$  equal to 5, 10, 20 and 40 ms, equivalent to 1, 221 222 2, 4 and 8 frames (Figure S1 is provided as supplemental material). Decreasing  $\Delta t$  from 40 to 10 223 ms caused an increase in the time-averaged  $u_y$  and  $u_x$  values. Further decreasing  $\Delta t$  from 10 to 5 224 ms led to little variation in either  $u_y$  or  $u_x$ , meaning the true maxima of velocity were captured at a time step of around 10 ms. Therefore, a time step  $\Delta t$  of 10 ms was chosen for the PIV analyses to 225 avoid positional errors associated with reducing the time step to very low values (Gollin et al., 226 227 2017).

The seeding density was approximately five tracers inside an interrogation window for both 228 tests (as shown in Figure S2 in the supplemental material) which is within the optimal range to 229 230 achieve a successful correlation and minimum random error (Thielicke, 2014). The seed image 231 size  $d_{\tau}$  was estimated as the width of the autocorrelation peak of a typical set of interrogation 232 windows (Michaelis et al., 2016; Patil & Liburdy, 2013). The autocorrelation peak width was calculated using the  $e^{-2}$  width. The resulting widths were 3.57±0.72 pixels for the test with the 233 234 spherical beads and 3.27±0.81 pixels for the test with angular particles (Figure S3). Both sizes lie 235 in the range of the tracer image diameter to achieve optimal measurements using the window 236 deformation algorithms in PIVlab (Thielicke, 2014).

# 237 *3.5.* Boundary flow field on a single plane

Figure 3 shows a typical flow field across the whole permeameter for a sample of beads, 238 239 considering three sub-volumes in the left, middle and right, respectively. The PIV analyses performed here show how the rigid lateral boundaries of the permeameter can disrupt the particle 240 241 packing, leading to some areas of large flow velocity in comparison to the mean, for example with 242 the high flow at the left boundary of Figure 3(a) compared to (b) and (c). In this preliminary 243 examination of the flow, an image mask was manually applied to the particle positions to exclude them from the fluid flow analysis. In contrast, for the following analyses focused on volumes at 244 245 the centre of the permeameter, the masks were automatically determined from image processing.

246

# 247 **4. Image Processing**

### 248 4.1. Image segmentation

249 Figure 4(a) shows a typical grey-scale image of a plane from sample Beads-U, illuminated by the laser. As shown in the schematic diagram at the top of the image, the finite laser thickness 250 251 leads to non-uniform grey values because particles can partially fill the laser beam. This is similar 252 to the partial volume effect associated with microCT images and consequences for image quality 253 are related to the laser thickness. The histogram of grey values of the image as shown in Figure 254 4(b) indicates there is no clear separation between the grey values for the particles and the pore-255 space. The distance between the scanning planes determines the image resolution in the z-direction, 256 i.e. the effective voxel length in the z-direction is 1 mm. Furthermore, the laser sheet creates linear streaks or shadows in the direction of the laser, with grey values that can be similar to that of 257 258 particles. In previous studies, the 3D pore space was reconstructed by identifying the centre and

radius of each spherical particle from 2D slices (Huang et al., 2008; Thaker et al., 2019) rather
than considering the 3D dataset directly. This shape-matching approach cannot be used for samples
with irregular-shaped particles.

262 Image segmentation of granular materials classifies each pixel as being either within a particle 263 or within the pore-space. We explored three approaches to segment the images, and Figure 5 264 presents the results of each of these methods applied to three representative slices. The first approach is threshold segmentation which classifies all pixels with a grey value lower than a 265 specified threshold as being in the particle phase and the remaining in the pore phase. The threshold 266 267 can be automatically determined by Otsu's algorithm based on the grey value histogram, as shown in Figure 4(b) (Otsu, 1979). The Otsu-threshold segmentation method incorrectly classified some 268 269 linear shadows created by the laser as being in the particle phase.

270 The other two methods considered, namely the trainable Weka (Waikato Environment for 271 Knowledge Analysis, Arganda-Carreras et al., 2017) and the U-Net (Ronneberger et al., 2015), are 272 based on artificial intelligence. Artificial intelligence segmentation approaches learn from 273 manually segmented images to define a pixel-wise classifier which labels each pixel as being in 274 either the particle or pore phase. The trainable Weka algorithm was developed in the open-source 275 software platform Fiji (Schindelin et al., 2012). When compared with the Otsu threshold, this 276 method improved the segmentation quality to some extent, but it could not completely remove the laser-induced linear shadows. Finally, the U-Net algorithm proved to be more robust in 277 segmentation, producing smooth particle-pore interfaces and no linear shadows, in contrast with 278 279 the other two methods. The segmented results from U-Net have smooth particle surfaces, no internal voids in the particles and eliminate all linear artefacts induced by the laser, which is 280 important for constructing CFD models. U-Net performs segmentation based on both grey values 281

and morphological patterns, e.g., edges, curvatures, and spheres. The U-Net package was
implemented in Tensorflow and Keras following the U-Net architecture proposed by Ronneberger
et al. (2015).

285 The U-Net segmentation procedure can be divided into three major steps: (a) data preparation 286 for training; (b) U-Net training; and (c) new image segmentation (Figure 6). The U-Net 287 architecture requires an image dimension of 512×512. Therefore, the images were scaled from 1280×800 pixels to 512×512 pixels and scaled back after segmentation. Initially, eight images 288 289 were segmented by visual inspection. Data augmentation was performed to increase the diversity 290 of training data by shifting and rotating each annotated image to produce four images. Thus a total 291 of 32 images were obtained for training and validation. Then the U-Net algorithm was trained with 292 32 annotated images to define the classifier. The trained U-Net classification led to an accuracy of 293 about 93% for validation images and was used as a classifier to segment new images. The U-Net classification generated a grey-scale image in which the grey value of a pixel reflected the 294 295 possibility of that pixel being in a particle. A target porosity was specified to generate an 296 appropriate threshold grey-level value to binarize the output of the U-Net algorithm. This porosity was selected by considering the experimental whole-sample value. However, acknowledging the 297 298 sample heterogeneity, a parametric study was carried out considering a range of reasonable local 299 porosity values as discussed below.

### 300 *4.2. Three-dimensional pore structure reconstruction*

The slice-by-slice scanning method led to an in-plane pixel size of approximately 0.029 mm along the x- and y-axes, and an out-of-plane distance of 1 mm along the z-axis. Therefore, we applied a scaling to the output from U-Net to reconstruct a three-dimensional volume with an

304 identical voxel size of 0.1 mm along all directions. Figure 7 shows the effect of upscaling along 305 the z-direction with three different interpolation methods. The scaling without interpolation results 306 in a stepped particle surface, while both interpolation methods provide relatively smooth particle 307 surfaces. The bilinear interpolation is adopted in this study. Finally, we binarized the scaled three-308 dimensional images with a threshold value to reach the porosity value determined experimentally. 309 The threshold value was determined from the linear relationship between the threshold value and 310 the resulting porosity. Three levels of porosity were used to reconstruct the pore topology to 311 investigate the influence of porosity on the CFD results.

312 We performed marker-based watershed labelling to identify individual particles from three-313 dimensional binary images. The image processing steps involved in labelling particles are: (a) 314 construct a distance map representing the distance from a pixel to its closest particle surface; (b) 315 use marker identification based on the H-Maximum algorithm (Soille, 2013) on the distance map; 316 (c) implement marker-based watershed segmentation using the markers and distance map. A more detailed description of this marker-based watershed segmentation approach can be found in Zhao 317 318 et al. (2015). Figure 8 illustrates the labelling results on typical 2D slices for beads and angular particles. The particles are less regular on x-z planes than on x-y planes. This is mainly due to the 319 320 finite step distance during the slice-by-slice scanning along the z-axis.

A marching cubes algorithm was used to generate triangular surface meshes from the voxel assembly representing individual particles (Lorensen & Cline, 1987). The surface meshes of individual particles were cleaned, simplified and smoothed with GMSH, an open-source mesh generator (Geuzaine & Remacle, 2009). Finally, the surface meshes of all particles were combined into a single file with individual particles represented by a unique label. Figure 9(a) and (b) show 326 the three-dimensional views of the particle packings in the scanning region for the samples with 327 spherical beads and angular particles, respectively.

328

# 329 5. Computed Fluid Dynamics (CFD) Simulation

### 330 5.1. Governing equation and numerical method

For the fully saturated conditions assumed here, flow through the pore space is governed bythe incompressible Navier-Stokes equations formulated as:

$$\rho_f\left(\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u}\right) = -\nabla p + \mu \nabla^2 \boldsymbol{u}$$
(Eq. 1)

$$\nabla \cdot \boldsymbol{u} = 0$$

(Eq 2)

where  $\boldsymbol{u}$  is the velocity vector, and p is the pressure. In the steady-state,  $\partial \boldsymbol{u}/\partial t = 0$ . Here the Navier-Stokes equations were solved using the Semi-Implicit Method of Pressure Linked Equations (SIMPLE) algorithm in the open-source CFD toolbox OpenFOAM (OpenFOAM Foundation, 2019). The SIMPLE algorithm is a steady-state solver for incompressible flow. The CFD analysis provides the velocity and pressure values at the centre of each CFD cell.

The simulation domain was discretized by the mesh generation algorithms available in OpenFOAM, i.e., BlockMesh and SnappyHexMesh. BlockMesh decomposes the simulation domain into blocks, while SnappyHexMesh takes the surface mesh defining the pore structure and chisels it with the geometry defined by the combined surface mesh file. We applied localized refinement at the particle surface, which increased the mesh densities close to the particle-particle contacts in particular. This created CFD meshes with around 3.5 million cells. Figure 9(c) and (d) show typical CFD meshes of pore space for spherical beads and angular particles, respectively. 345 In all simulations, a constant pressure boundary condition was applied at both the inlet (17 Pa) 346 and outlet boundaries (0 Pa). A 'slip' condition was applied to the four lateral boundaries so that the velocity component normal to each of these boundaries was set to be zero while the tangential 347 348 velocities remained unconstrained. A 'no-slip' boundary condition was applied to the particle surfaces so that the velocities normal and tangential to the surface were set to zero. These boundary 349 conditions are similar to those applied in the CFD analyses by Taylor et al. (2016). They do not 350 351 capture the heterogeneity of the pressure and velocity distributions that exist on the boundaries of sub-volumes in experiments. However, the flow velocity data available from the experiments are 352 353 restricted to 2D and limited to 26 discrete vertical planes. A valid CFD analysis requires 354 conservation of mass (adherence to continuity) in the model in all three dimensions. Consequently, it was not possible to use the experimental data to apply non-uniform velocity fields along the 355 356 boundary to the simulation domain.

The normal and shear stresses on the particle surface were determined from the flow velocity and pressure fields. Each particle surface was discretized into surface elements. Then, the flowinduced force and moment on individual particles were calculated by integrating normal pressure and viscous shear stresses over all elements on the particle surface:

$$\boldsymbol{F}_{\boldsymbol{p}} = \sum_{i=1}^{N_e} \rho p_i A_i \boldsymbol{n}_i \tag{Eq. 3}$$

$$\boldsymbol{F}_{\boldsymbol{v}} = \sum_{i=1}^{N_e} \mu \boldsymbol{R}_{dev} A_i \tag{Eq. 4}$$

where  $N_e$  is the number of elements covering the particle surface,  $\rho$  is the fluid density,  $p_i$  is the kinematic normal pressure,  $A_i$  and  $n_i$  are the patch area and normal vector,  $\mu$  is the fluid dynamic viscosity, and  $R_{dev}$  is the deviatoric stress tensor. The integration was performed using the in-built function, 'forces', in OpenFOAM (OpenFOAM Foundation, 2019).

## 365 5.2. Validation with regular packings

366 The CFD simulation data are inherently dependant on the mesh density (cell size) (e.g. Knight 367 et al. 2020). The sensitivity of the fluid-particle interaction forces obtained from the CFD 368 modelling approach adopted here to the mesh density was examined by considering the data in 369 Zick & Homsy (1982) for simple cubic (SC) and face-centred cubic (FCC) packings of uniformly 370 sized spheres. Following Knight et al (2020), the models exploited geometric symmetry to reduce the calculation cost. As before, a specified pressure was applied at the inlet and outlet, while 'cyclic' 371 372 boundary conditions were applied to the four lateral boundaries. The sphere centroids were placed on a fixed lattice, and the particle sizes were changed to reach different packing densities; e.g. the 373 374 particle diameter was increased from 4.4 mm to 4.9 mm in the FCC packings to achieve porosity between 0.495 and 0.303. The fluid-particle interaction coefficient,  $\bar{F}_{f \to s}$ , is the fluid-particle 375 interaction force normalized by Stokes drag force  $F_{f \to s}^s$ : 376

$$F_{f \to s}^s = 3\pi\mu D|u| \tag{Eq. 5}$$

$$\bar{F}_{f \to S} = F_{f \to S} / F_{f \to S}^S$$

(Ea 6)

where *D* is the particle diameter, *u* is the superficial flow velocity, and  $F_{f \to s}$  is the fluid-particle interaction force, which includes both the pressure and viscous terms.

The fluid-particle interaction coefficient increases with reduced packing porosity, as shown in Figure 10(a). The results from CFD simulations are consistent with the Zick and Homsy solutions and the results from Immersed Boundary Method (IBM) obtained by Knight et al. (2020). The 382 CFD results are mesh dependent. As shown in Figure 10(b) and (c), the agreement between the 383 fluid-particle interactions obtained from these CFD simulations and the Zick and Homsy data,  $|\bar{F}_{f\to s} - \bar{F}_{f\to s}^{ZH}|/\bar{F}_{f\to s}^{ZH}$ , improves with increasing mesh density,  $D/d_m$ , where D is the particle 384 385 diameter, and  $d_m$  is a characteristic mesh element size. At the same  $D/d_m$ , the relative error 386 increases with sample density. The relative errors for most samples were smaller than 5% at a  $D/d_m$ 387 of 40. The results obtained from the unstructured mesh CFD analyses by Knight et al. (2020) show 388 a similar influence of mesh density on relative error for drag estimation. The average ratio between 389 particle diameter and mesh element size was chosen to be 40 for the permeameter simulations.

390

# **6. Results**

The 2D-PIV measurements can only provide the components of flow velocities in the plane of the laser, i.e. along the x- and y-directions. Within this plane, the distance between PIV data points is around 0.5 mm, which is much larger than the CFD mesh size. Therefore, the CFD velocity fields were interpolated to the centre of the PIV interrogation regions to allow a direct comparison between the PIV and CFD results. The Reynolds number in this study is around one, which indicates a laminar flow condition. We normalized the velocity values by the mean vertical velocity either on each vertical slice ( $\bar{u}^s$ ) or the mean value in each sub-volume ( $\bar{u}^v$ ).

For each sub-volume, the PIV analysis was performed on 26 x-y planes at 1 mm intervals. The x-y planes were referred with their z coordinates from 0 mm to 25 mm. The CFD domain is slightly smaller than the PIV domain and has 24 x-y planes (z = 1 to 24 mm) to reduce the effects of upscaling on boundary slices (Figure 7). The sub-volume has about six particles along the xdirection and four particles along the y-direction, and there are about 20 particles completely inside each sub-volume.

### 405 *6.1. Permeability estimation*

406 Table 3 shows the experimental measurements for each sub-volume. Each sub-volume is named by the particle type, e.g. spherical (Beads) and angular (Ang), followed by the position, e.g. 407 upper (U) and lower (L). The overall packing porosity, n, permeameter cross-section area,  $A_{Exp}$ , 408 and flow rate,  $Q_{Exp}$ , were measured during each permeameter test. Local manometer readings were 409 used to identify the hydraulic gradient for the experiments, and the two sub-volumes in the angular 410 particle sample had slightly different hydraulic gradients  $i_{exp}$  due to the inhomogeneous packing. 411 Seepage flow rates were determined from experimental measurements  $(u_{seen}^{Exp})$ , PIV analysis  $(u_{seen}^{PIV})$ 412 and CFD simulations  $(u_{seep}^{CFD})$ . 413

414 Figure 11 compares the permeability values estimated by the three types of seepage velocities. In general, the permeability values estimated by PIV analysis  $(k^{PIV})$  are smaller than the values 415 estimated from the experimental measurements  $(k^{Exp})$ . This is unsurprising as the PIV analysis 416 was performed over central sub-volumes, while the pump injection rate measures the cross-section 417 of the permeameter, including the larger voids commonly encountered at the side walls (Figure 3). 418 419 In addition, the sub-volumes for Ang show smaller permeabilities than the sub-volumes for Beads. For  $k^{Exp}$  the sub-volume Ang-U has a higher permeability than for Ang-L due to the different 420 hydraulic gradient as measured using the manometers, while there was no evident difference in the 421 sub-volumes of the Beads sample. In Figure 11(a) the  $k^{CFD}$  data were obtained using the overall 422 experimental porosities, i.e. n = 0.38 and 0.36 in the CFD simulations for Beads and Ang samples, 423 respectively. Perhaps surprisingly, the permeability values estimated by CFD simulations,  $k^{CFD}$ 424 (grey data points), are similar across the four sub-volumes, with only a slight decrease for the Ang 425 sample compared to the Beads. This means that, while the permeabilities estimated for CFD and 426

427 PIV in the Beads sub-volumes are quite close, for the angular sample,  $k^{CFD}$  measurements are 428 approximately twice that of  $k^{PIV}$ .

The differences between experimental and numerical permeabilities could be caused by (a) 429 local porosity variations, (b) CFD boundary effects, or (c) PIV velocity measurement errors. Figure 430 11(b) illustrates the sensitivity of the  $k^{CFD}$  results to porosity by considering three limiting 431 plausible porosity values. For Beads-U,  $k^{CFD}$  agrees with both  $k^{Exp}$  and  $k^{PIV}$  if local porosity is 432 changed from 0.38 to 0.40. For Ang-U,  $k^{CFD}$  agrees with  $k^{Exp}$  and  $k^{PIV}$  if the local porosity is 433 changed from 0.36 to 0.31 and 0.29, respectively. However, the segmented images seem to be 434 inconsistent with the grey-value images due to the large porosity change (Figure S4 in the 435 supplementary material). Furthermore, the variation in porosity had only a limited influence on the 436 437 flow field distributions. Potential PIV velocity measurement errors were also investigated by 438 changing the framerate. However, this did not lead to a noticeable change. A definitive, precise explanation for the inconsistency in the permeability values could not be determined. 439

# 440 6.2. Flow fields – contour plots

The normalized flow fields obtained from PIV and CFD analysis within a typical x-y plane for 441 the Beads-U sub-volume are in good agreement, as shown by the normalized horizontal velocity 442  $\bar{u}_x^s$  and vertical velocity  $\bar{u}_y^s$  in Figure 12. The heterogeneity in the packing leads to concentrated 443 444 flow paths for vertical flow at some large voids, e.g. close to the left bottom corner. The horizontal 445 velocity is determined by the local pore alignment relative to the macro-scale flow direction. The 446 lateral boundaries assumed in the CFD models prohibit horizontal flow, so the flow patterns at the 447 side boundaries differ. For example, the physical test data indicate a relatively large horizontal flow close the left boundary in Figure 12(a) which is not captured in the CFD model in Figure 448

449 12(b). The difference in the boundary conditions also influences the vertical velocity values in this 450 region. The vector plots of flow fields on three x-y planes are shown in Figure 13 to further 451 demonstrate the similar patterns revealed by PIV and CFD estimations. Again, the lateral boundary 452 conditions inhibit horizontal flow in the CFD model.

453 The flow velocities on four x-y planes in the Beads-U sub-volume were analysed statistically, as shown in Figure 14. The horizontal normalised velocity  $\bar{u}_x^s$  tends to form a Laplace distribution 454 with a mean velocity around zero (Figure 14(a)). While the distributions obtained from the PIV 455 456 analyses are similar for the four planes considered, the two CFD distributions with z=1 mm and 457 24 mm tend to have a higher proportion of data points with a velocity close to zero, due to the lateral boundary effect experienced at the front (z = 1 mm) and back (z = 24 mm) of the studied 458 volume. The vertical normalised velocity  $\bar{u}_y^s$  tends to form a half Laplace distribution (Figure 459 14(b)). Similarly, the planes close to the front or back lateral boundary in the CFD simulation (z= 460 461 1 mm and 24 mm) have a higher proportion of velocity close to zero. The cumulative distributions in Figure 14(c) and (d) show a good agreement between PIV and CFD results. 462

463 The pore topology is intrinsically correlated with particle morphology and granular material packing/fabric. The flow fields on three x-y planes of the Ang-L sub-volume show the flow 464 patterns that are distinct from those developed in the Beads-U sub-volume (comparison between 465 Figure 15 and Figure 13). Some flow channels are straight rather than converging-diverging due 466 to the flat surfaces of angular particles, as indicated by arrows. The difference seems to be more 467 obvious for the angular particle sample than for the beads sample. However, the overall 468 distribution of flow velocity in the angular particles sample is very similar to that of the beads 469 470 sample, as shown in Figure 16. Previous studies have indicated that the flow velocity distribution depends on packing density (Rong et al., 2013). Further tests are needed to investigate the influence
of particle shape on the flow velocity distribution.

The mapping of the CFD data onto the PIV grid allows spatial variation of the difference 473 474 between the two datasets to be examined, as shown in Figure 17(a) and (b). While the data in Figure 12 showed the similarity of the flow patterns, there are large differences between the 475 476 normalized velocity intensities. Figure 17(c) and (d) show the cumulative distributions of the 477 velocity difference values for five x-y planes. The difference mainly lies between  $\pm 50\%$  and  $\pm 100\%$  of the mean seepage velocity on each slice for horizontal and vertical velocity, 478 respectively. Perhaps unsurprisingly, the planes closest to the lateral boundaries (z=1 or 24 mm) 479 have a higher velocity difference. 480

# 481 6.3. Mean flow rate on slices

482 Here, the mean velocity on each x-y plane is normalized by the seepage velocity in each sub-483 volume. The normalized vertical velocity on each plane varies between 0.5 and 1.5, as shown by Figure 18(a). The PIV and CFD data exhibit similar patterns of variation in  $\langle \bar{u}_{\nu}^{\nu} \rangle$  along the z-axis. 484 In the CFD analyses, the lateral boundaries prohibit out-of-plane flow and lead to low velocity 485 values along z, as shown by the shaded area in Figure 18(b). However,  $\langle \bar{u}_z^{\nu} \rangle$  increases to the 486 expected level after about 3 mm ( $\sim D/2$ ) from the lateral boundary. The heterogeneity of the pore 487 488 structure and relatively small sub-volume leads to a large variance of the plane-based porosity 489 (Figure 18(c)). For example, the plane-based porosity for the Beads-U sub-volume (n=0.38) varies 490 from 0.25 to 0.5.

The CFD analyses provide 3D data, enabling analysis of the velocity distribution in horizontal
 x-z planes perpendicular to the flow direction. As expected, the variance of the mean vertical

493 velocity  $\langle \bar{u}_{y}^{\nu} \rangle$  on x-z planes is inversely correlated to the plane porosity due to the fluid continuity 494 (Figure 19(a) and (b)). Where the porosity in the x-z plane is lower,  $\langle \bar{u}_{y}^{\nu} \rangle$  is higher so that overall 495 flow rate is the same for each x-z plane in line with the principle of mass conservation. The pressure 496 dissipation is higher at the lower porosity plane, as shown in Figure 19(c).

# 497 6.4. Fluid-particle interactions

Each sub-volume contains around twenty particles that do not intersect the boundaries. Figure 20 shows the vector plots of the fluid-particle interaction coefficients  $\overline{F}_{f \to s}$  (Equation 6) projected onto x-y planes for four sub-volumes. The magnitudes of  $\overline{F}_{f \to s}$  have a large variance, especially for angular particles. The directions of  $\overline{F}_{f \to s}$  slightly deviate from the flow direction – the mean deviation angle equals 16°. The variance of  $\overline{F}_{f \to s}$  arises mainly from the heterogeneous flow fields, resulting from local packing and irregular particle morphologies.

Figure 21(a) shows the distribution of the fluid-particle interaction coefficient, which varies approximately from 50 to 140 for beads and from 50 to 240 for angular particles. The mean value of  $\overline{F}_{f \to s}$  is influenced by the different packing densities, with the angular particle sample having a slightly higher packing density than the beads sample. Figure 21(b) shows the fluid-particle interaction coefficients normalized by their mean values. Clearly, the sample with angular particles has a higher variance than the spherical beads sample. This variance may arise from packing density or particle shape difference.

The fluid-particle interaction is contributed by two components, i.e. a viscous component due to skin friction and a pressure component due to the pressure gradient. In dense packings, the pressure component of fluid-particle interactions dominates the fluid-particle interaction, while the viscous component accounts for about 20% on average, as shown in Figure 22(a). Spherical beads tend to experience a slightly higher ratio of the viscous component to pressure component than angular particles. Figure 22(b) shows the deviation angle of fluid-particle interactions from the flow direction, i.e.  $\theta_d = \arctan(\bar{F}_{f \to s, xz}/\bar{F}_{f \to s, y})$ . Most particles have a deviation angle between 0° and 30°.

519

# 520 **7. Conclusions**

This study investigated pore-scale seepage in granular packings with the combined 521 522 experimental and numerical methods. Permeameter tests were performed with transparent soils consisting of spherical and angular particles. PIV analysis quantified 2D flow fields inside granular 523 524 packings on multiple planes. We adopted a series of image processing techniques to reconstruct 525 the 3D pore topologies from the slice-by-slice scanning images. Pore-scale CFD analysis was performed on reconstructed volumes to obtain both flow fields and fluid-particle interactions. The 526 527 fluid-particle interactions obtained by CFD simulations were validated with existing results on regular particle packings. The conclusions are summarised as follows. 528

529 PIV analysis can quantify the flow field for two-dimensional planes. The random packing of 530 particles leads to preferential flow paths at larger voids (e.g. close to boundary wall). Spherical 531 particles tend to form converging and diverging flow paths, while angular particles with flat 532 surfaces form straight channels. The interplays between local particle arrangement, particle shape 533 and pressure gradient determine the heterogeneous pore-scale flow fields.

The slice-by-slice images containing pore structure information were obtained by illuminating the transparent soils at multiple locations with a sheet laser. An artificial intelligence algorithm provided good image segmentation results for the images with poor contrast and artefacts. The flow fields obtained from CFD analysis on the reconstructed pore structure show a good agreement with PIV results. Similar patterns were obtained for the contour plots of flow fields, flow vector plots and velocity magnitude histograms. This agreement demonstrates the successful implementation of the three-dimensional pore structure reconstruction methods. However, while there is good agreement between the average flow fields, the local differences in flow field data are more significant.

This work supports the development of systems with thinner lasers (including the requisite safety considerations) and exploiting recent advances in automated systems for macro photography to reduce the observed partial volume effects and improve the resolution orthogonal to the scanning planes (i.e. in the z-direction considered here).

The CFD results have a higher resolution in comparison with the PIV results and produce three-dimensional velocity values. However, the analyses tend to have side boundary effects. The comparison between CFD and PIV results indicate the side boundary effects are usually constrained within a half particle diameter region. The point-by-point comparison of CFD and PIV results was performed after downscaling the CFD results. The normalized velocity difference remains large, even though the overall distribution of CFD and PIV flow fields are similar.

The fluid-particle interactions obtained from fully resolved CFD analysis are consistent with 553 554 previous numerical solutions. The fluid-particle interactions obtained the permeameter model tests have a large variance, especially for angular particles. For relatively dense packings, viscous drag 555 contributes to a small fraction of the total fluid-particle interaction. The fluid-particle interaction 556 557 slightly deviates from the injection direction. However, for this study, the number of particles in each CFD model was relatively small (around twenty), and the beads and angular particles samples 558 have slightly different packing density. Therefore, the fluid-particle interaction results should be 559 560 further investigated to elaborate on the particle shape effects.

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562 Figure 1. Schematic of the experimental set up.

563 Figure 2. Images of experimental setup: (a) Permeameter cell partially filled with oil; (b) Beads

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- 633 V2. Video of an illuminated section in the angular sample showing the movement of tracers

# Nomenclature

A <sub>Exp</sub>	permeameter cross section area
A <sub>i</sub>	area of CFD mesh element
$d_m$	characteristic mesh size
$d_s$	seed particle diameter
D	diameter of beads and angular particles
D <sub>I</sub>	interrogation window size
$F_{f \to s}^s$	stokes drag force
$\overline{F}_{f \to s}$	fluid-particle interaction coefficient
$\overline{F}_{f \to s, xz}$	projection of fluid-particle interaction coefficient on x-z plane
$\overline{F}_{f \to s, y}$	projection of fluid-particle interaction coefficient on flow direction – y axis
$\overline{F}_{f \to s}^{ZH}$	fluid-particle interaction coefficient from Zick and Homsy solutions
F <sub>p</sub>	pressure component of fluid-particle interaction force
$F_v$	viscous component of fluid-particle interaction force
<b>k</b> <sup>CFD</sup>	hydraulic permeability determined through CFD analysis
k <sup>Exp</sup>	hydraulic permeability determined through experimental measurements
k <sup>PIV</sup>	hydraulic permeability determined through PIV analysis
n	packing porosity
n <sub>i</sub>	normal vector of CFD mesh element
N <sub>e</sub>	number of CFD mesh element on particle surface
р	fluid pressure
$p_i$	kinematic normal pressure on CFD mesh element

- *R*<sub>*dev*</sub> deviatoric stress tensor
- *Stk*<sub>s</sub> Stokes number for seed particles
- $\Delta t$  time step used for PIV analysis
- *u* fluid velocity vector
- $u_x$  component of fluid velocity in the *x*-direction
- $u_y$  component of fluid velocity in the y-direction
- $u_z$  component of fluid velocity in the *z*-direction
- $u^s$  velocity magnitude normalized by mean seepage velocity on each slice
- $u^{\nu}$  velocity magnitude normalized by mean seepage velocity in each sub-volume
- $\langle u^{\nu} \rangle$  mean velocity on slice normalized by mean seepage velocity in each sub-volume
- $u_{seep}^{Exp}$  seepage velocity determined through experimental measurements
- $u_{seep}^{PIV}$  seepage velocity determined through PIV analysis
- $u_{seep}^{CFD}$  seepage velocity determined through CFD simulations
- $v_{seep}$  seepage flow velocity
  - $\mu$  fluid dynamic viscosity
  - $\rho$  fluid density
  - $\rho_s$  seed particle density
  - *v* fluid kinematic viscosity
- $\theta_d$  deviation angle of fluid-particle interaction from the fluid injection direction

635

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## 756 Table 1. Particle and fluid properties

	Particle	Density	Refractive	Viscosity	
	diameter [mm]	[g/cm <sup>3</sup> ]	index	Kinematic [mm <sup>2</sup> /s]	Dynamic [Pa·s]
SiLibeads Glass beads Type P Borosilicate	$7.5 \pm 0.03$	2.23	1.46 (*)	-	
Duran® angular particles	6.7 – 9.5	2.23	1.47 (at 21°C)	-	
Cargille immersion fluid	-	0.846	1.47 (at 25°C)	16 (at 25 °C)	0.0135
Microsphere fluid seeding particles	0.005 - 0.030	0.750	-	-	

(\*) The measurement temperature for the refractive index value was not given on the material certificate.

A sensitivity analysis to temperature was conducted to achieve the optimum optical transparency with the
immersion fluid.

763 Table 2. Sub-volume dimensions

Sub-volume	Dimensions, $x \times y \times z$ [mm <sup>3</sup> ]			
Beads-U	37.4 × 23.4 × 25			
Beads-L	40.4 × 25.3 × 25			
Ang-U	38.5 × 24.0 × 25			
Ang-L	38.5 × 24.0 × 25			

Sub-volume	п	i <sub>Exp</sub>	AExp [cm <sup>2</sup> ]	Q <sub>Exp</sub> [ml/s]	u <sup>Exp</sup> [mm/s]	u <sup>PIV</sup> [mm/s]	u <sup>CFD</sup> [mm/s]
Beads-U	0.38	0.086	100	30.3	8.0	7.1	6.8
Beads-L	0.38	0.086	100	30.3	8.0	5.7	6.2
Ang-U	0.36	0.143	100	28.5	7.9	4.5	6.0
Ang-L	0.36	0.114	100	28.5	7.9	4.5	5.9

Table 3. Experimental and numerical measurements for each sub-volume

Figure 1. Schematic of the experimental set up.



Figure 2. Images of experimental setup: (a) Permeameter cell partially filled with oil; (b) Beads sample illuminated by laser sheet; (c) Angular particles sample illuminated by laser sheet; (d) top view of the laser sheet.



Figure 3. Flow fields in the (a) left, (b) middle and (c) right for the permeameter with beads.



Figure 4. (a) Typical grey-scale image in Beads-U sub-volume, z = 0 mm. (b) Histogram of grey values. Inset in (a) shows that the non-uniform intensity is a consequence of the finite laser width.



Figure 5. Segmentation results for three typical slices in Beads-U sub-volume using three different segmentation methods: threshold segmentation with Otsu's threshold, trainable Weka segmentation, and U-Net segmentation. Note: dashed circles indicate the artifacts produced by inaccurate segmentation.



Figure 6. U-Net segmentation procedure for Beads-U sub-volume: (a) Step-1: prepare training and validating data sets; (b) Step-2: train U-Net algorithm; (c) Step-3: apply trained U-Net as a classifier for segmenting new images.



Figure 7. Upscaling along *z*-direction on the U-Net classified image for Beads-U sub-volume: (a) Unscaled image data; (b) Image obtained by scaling without interpolation; (c) Image obtained by scaling with bilinear interpolation; (d) Image obtained by scaling with bicubic interpolation.



Figure 8. Labelled images with particles represented by different colours for Beads-U sub-volume on (a) x-y plane and (b) x-z plane and Ang-U sub-volume on (c) x-y plane and (d) x-z plane.



Figure 9. Three-dimensional views of the combined surface meshes for (a) Beads-U sub-volume and (b) Ang-U sub-volume. Note: colour is used to distinguish the surfaces of individual particles. Hexahedron meshes which discretize pore structure for CFD simulation for (c) Beads-U sub-volume and (d) Ang-U sub-volume.



Figure 10. Verification of CFD modelling approach: (a) Confirmation of ability to capture the influence of porosity on the fluidparticle interaction coefficient  $\overline{F}_{f \to s}$ , dashed lines indicate a curve fit to the Zick & Homsy (1982) data; (b) Mesh dependence of  $\overline{F}_{f \to s}$  for SC packings; (c) Mesh dependence of  $\overline{F}_{f \to s}$  for FCC packings. The results predicted by the Immersed Boundary Method (IBM) with a regular grid and from fully resolved CFD using an unstructured meshes from Knight et al. (2020) are included in (a) and (c), respectively.



Figure 11. (a) Hydraulic permeability values predicted by experiments, PIV and CFD measurements. (b) Influence of porosity on hydraulic permeability as estimated by CFD modelling for Beads-U and Ang-U sub-volumes. The prediction results from Kozeny-Carman Equation (KC Eq.) is included in (b).





Figure 13. Comparison of the PIV and CFD flow fields in Beads-U sub-volume on three slices with z= 1, 8 and 16 mm. Velocity vector length is normalized by seepage velocity.



Figure 14. Cumulative distributions of flow velocity at four vertical planes in Beads-U sub-volume obtained from PIV and CFD results.



Figure 15. Comparison of the PIV and CFD flow fields in Ang-L sub-volume on three slices with z = 1, 8 and 16 mm. Velocity vector length is normalized by seepage velocity. Arrows indicate narrow flow paths.



Figure 16. Cumulative distributions of flow velocity at four vertical planes in Ang-L sub-volume obtained from PIV and CFD results.



Figure 17. Difference between PIV and CFD flow fields for the vertical slice with z = 16 mm in Beads-U sub-volume: (a) horizontal velocity; (b) vertical velocity. The cumulative distributions of PIV and CFD difference for (c) horizontal velocity and (d) vertical velocity on five typical slices in Beads-U sub-volume.



Figure 18. Variation of the mean velocity values obtained from PIV and CFD results and the slice porosity on x-y planes parallel to flow direction.



Figure 19. Variation of mean vertical velocity, porosity and hydraulic gradient on x-z planes perpendicular to flow direction predicted by CFD simulations.



Figure 20. Projection views of drag force vectors for the particles that are not intersecting with boundary walls.



Figure 21. Cumulative distributions of (a) fluid-particle interaction coefficients for beads and angular particles and (b) the normalized fluid-particle interaction coefficients.



Figure 22. Distributions of (a) the ratio between pressure and viscous drag components, and (b) the angle between fluid-particle interaction and flow direction.



Figure S1. Example of the effect of time resolution of PIV analysis on the estimate of the time averaged component (a)  $u_x$  and (b)  $u_y$ . The velocities are estimated along the yellow dashed lined shown in the inset of (a).



Figure S2. Distribution of the number of tracers for a subsets of interrogation windows (32 x 32 pixels) for (a) beads and (b) angular particles.



Figure S3. Autocorrelation function for a subsets of interrogation windows (32 x 32 pixels) for (a) beads and (b) angular particles. Histogram of autocorrelation peak width for (c) beads and (d) angular particles.



Figure S4. (a) Typical slice of Ang-U processed by U-Net, and the binarization results at different porosity values (b) 0.31, (c) 0.29, and (d) 0.27.

