Title: Sub-Particle-Scale Investigation of Seepage in Sands

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ABSTRACT: While seepage poses significant challenges to many geotechnical projects and hydraulic conductivity is a key soil property, fundamental pore-scale understanding of water flow in soil is poor. The seepage velocities considered in geotechnical engineering are area-averaged flow rates and their relation to the actual fluid velocity is unclear. Some of the predictive formulae for sand currently used in engineering practice were developed using simplified particle-scale analytical models whose validity is not well-established. Recent advances in modelling and imaging enable these uncertainties associated with seepage to be addressed and this paper proposes a first principles simulation approach in which flow in the void space is modelled by applying Computational Fluid Dynamics (CFD) to void geometries obtained using X-ray micro-Computed Tomography (microCT). The model was verified by comparison with hydraulic conductivity data from laboratory permeameter tests on the same materials. The data generated provide significant sub-particle-scale insight into fluid velocities and head loss. The results are used to show that existing models for predicting hydraulic conductivity struggle to account for the full range of particle variables and fail to explain the true governing variables, which relate to the micro-scale properties of the void space.

Keywords: Seepage, Sands, Permeability, Numerical modelling, Laboratory tests.

International Geotechnical Classification System: D04 (seepage), E13 (computer models)

1. INTRODUCTION

In seepage analyses geotechnical engineers typically consider soil as a porous continuum and apply Darcy's law. The importance of understanding the fundamental seepage process is emphasized in textbooks including Harr (1990) and Mitchell & Soga (2005). This contribution improves upon the schematic diagrams and analytical models proposed in these texts by using high resolution 3D images and computational fluid dynamics (CFD) (with a discretization resolution scale that is smaller than the particle size) to quantify the fluid flow within the void space of sands. The insight that can be obtained from this approach can advance understanding of internal instability and filtration (Dallo & Wang, 2016; Kenney et al., 1985; Kézdi, 1979); ground improvement (Kim & Whittle, 2009); mechanical dispersion of contaminants (discussed in Fetter (1994) and Fitts (2012)); well development in in-situ permeability testing (Cashman & Preene, 2001); etc. This paper describes the experimental procedure to acquire microCT images; the pore-scale CFD simulations and model verification by comparison with laboratory permeameter tests. The data generated enabled an analysis of the local velocities and the fundamental mechanisms head loss in sand. The technique is applied to reassess the basis for the Kozeny-Carmen equation and other equations used to predict hydraulic conductivity (k) in geotechnical analysis.

2. ACQUISITION OF VOID TOPOGRAPHY

Specimen Preparation

Referring to Table 1 and Figure 3, four materials were considered to enable the influence of particle size distribution (PSD) and particle shape to be considered. For each material samples were prepared in a triaxial cell using the dry deposition method (Ishihara, 1993) and densified to approximately 50-70% relative density (based on the maximum and minimum void ratios achievable by this deposition method) by tapping the base of the cell. An air suction of approximately 30 kPa was applied to the top cap temporarily, to maintain sample integrity until the cell was assembled, then a 30 kPa cell air pressure was applied. To preserve the void structure and to produce samples small enough to allow high resolution imaging (Cnudde & Boone, 2013), triaxial samples were resin impregnated and sub-sampled as described in Fonseca et al. (2013). Referring to Figure 4(a), resin was drawn up from the base by elevating the resin container and applying a small air suction (≈1 kPa) at the top cap. The resin was allowed to cure for at least 24 hours before coring 9 mm central sub-

samples. To test repeatability, two separate triaxial samples were prepared for material Sand-Cu3, identified as [1] and [2], making a total of five samples.

MicroCT imaging

The 9 mm cores were scanned using a Nikon XT–H–225 microCT scanner at Queen Mary University London, using the scanning parameters given in Table 2. Image processing involved median filtering and threshold segmentation using the method proposed by Otsu (1979), to produce the 3D binary images shown in Figure 5 where each voxel is designated to be solid (grey in Figure 5) or void (transparent) depending on the level of X-ray attenuation.

The samples were inhomogeneous and so the PSDs were determined for each core using the microCT data following the approach detailed in Fonseca et al.(2012). Watershed segmentation of the particle phase was used to identify individual particles; using principle component analysis, the particle orientations were determined and used to define an orthogonal bounding box around each particle. The intermediate length of the bounding box was taken as the particle size for use in the PSD. For comparison, the points on Figure 3 denoted as "LAB D_{10} & D_{60}" indicate the particle sizes for 10% passing and 60% passing by mass, measured in the laboratory by dry sieving. These points show good agreement between the image-based particle sizes and conventional laboratory methods.The coefficient of uniformity, C_u ($=D_{60}/D_{10}$) was used to characterize each PSD.

Any approach to partition the continuous void space will be subjective. In the current study the were geometrically identified following the approach described in Taylor et al. (2015). Referring to Figure 6(d), the void space was segmented into discrete void regions using watershed segmentation. This process defines the void boundaries; the constriction diameters were then calculated as the local maxima of the distance map on the boundary surface; a post processing step is required to remove extraneous local maxima so that only meaningful constrictions are identified (full details are given in Taylor et al., 2015). Taylor et al. (2015) demonstrated that this approach gives results that are comparable with other geometric partitioning algorithms while having the advantages of greater adaptability for different materials and improved 3D visualization of constrictions. The size of voids and void constrictions (and hence the analyses discussed in this paper) are sensitive to the image processing methodology. Image processing parameters were selected based on the

recommendations by Taylor et al. (2015) and were kept consistent for the five samples analyzed in this study so that valid conclusions can be drawn as to how the void space and sub-particle flow regimes differ for these five samples.

Constriction size measurements for the five specimens are presented in Figure 3 as constriction size distributions (CSDs). These CSD curves demonstrate the effects of C_u and particle shape on constriction sizes, where a higher C_u results in a wider range of constriction sizes; and angular particles produce more constrictions at both the upper and lower ends of the constriction size range, compared to spherical particles.

3. COMPUTATIONAL FLUID DYNAMICS (CFD) SIMULATIONS

Model Development

CFD simulations were performed using the open source CFD solver OpenFOAM (Version 2.4.0, 2015) which has been used successfully in similar studies on porous rocks (Mostaghimi et al., 2013; Pereira Nunes et al., 2015; Piller et al., 2014; Raeini et al., 2012). OpenFOAM solves the conservation of mass and momentum equations iteratively over a finite volume mesh, using the Semi Implicit Method of Pressure Linked Equations, or SIMPLE algorithm (OpenFOAM Foundation, 2014; Raeini et al., 2012). The cell size used in the CFD simulations was one voxel. A 'no slip' boundary condition was applied at the particle surfaces, meaning that there was no flow across these boundaries and also the velocities along the boundary are zero. In contrast to coupled DEM studies either using CFD (e.g. Zeghal and El Shamy, 2004) or the lattice Boltzman technique (e.g.Galindo-Torres, 2013) to resolve the fluid flow, these simulations are not coupled, i.e. the transfer of momentum between particles and fluid is not considered and the particles are assumed to remain static under the fluid flow. Once the iterative solution has converged, the outputs are pressure and velocity values at the center of each mesh cell.

Finite volume meshes were generated by converting the voxelized binary images, shown in Figure 5, into 3D stereolithographic surfaces (.stl format) using the open source imaging software ImageJ (Rasband, 2012), then filling the void within this surface with a polyhedral mesh using the open

source graphical user interface HELYX-OS (Engys, 2015). Sub-volumes 400 × 400 × 400 voxels in size were analyzed, rather than the full images, so that mesh generation and convergence of the CFD solver could each be achieved within 24hrs on a desktop computer with 144GB of RAM. The length of these sub volumes was relatively small, approximately 5-7 times D_{50} (median particle diameter) and so to assess whether the sub-volumes were representative elementary volumes (REVs), void ratio variations were measured in cubic sub-volumes with varying sizes and at varying locations within the images. The variation in void ratio reduced as the sub-volume size increased from 100^3 to 400^3 voxels, but no significant improvement was achieved by a further increase to 500^3 voxels, supporting the use of 400^3 voxel sub-volumes as REVs. For four of the five sub-volumes, the void ratios were within $\pm$0.01 (≈ $\pm$2%) of the average for the full image, while for Sand-Cu3[1] the difference was +0.03 (≈ +6%). This difference in void ratio indicates that the Sand-Cu3[1] sub sample may not be representative of the average properties for larger samples, consequently the hydraulic conductivity of this sub sample should be higher than that of larger samples. Mostaghimi et al. (2013) found the REV for hydraulic conductivity measurements to be larger than that required to capture void ratio, hence comparison with laboratory permeameter measurements (discussed below) was used to demonstrate that the small sub-volumes were representative.

Before analyzing the microCT images, the OpenFOAM solver was validated using a synthesized 3D image of a periodically constricted tube (Figure 7(a)), with voxel size comparable to the microCT images. The velocity outputs from the CFD solution were interpolated to give values at the center of each voxel, producing the normalized values shown in Figure 7(b). Velocity values were typically within $\pm$2% of the analytical solution given by Sisavath et al. (2001) which was deemed acceptable, however values within 5 voxels of the inlet and outlet boundaries had errors up to $\pm$10% from the analytical solution. Figure 7(c) shows pressure values along the tube centerline and supports the earlier hypothesis (Figure 1(d)) that the gradient of pressure loss is significantly steeper at the constrictions.

Rajon et al. (2002) showed that voxelization can overestimate surface area by up to 50%, for 3D spheres. To minimize this error, which will impact CFD simulations, the void geometry was smoothed using the ‘smooth’ function in Rhino 5.0 (Robert McNeel & Associates, 2015), as shown for a single particle in Figure 8. Test images of voxelized spheres (Figure 8(c)) showed that the smoothing

process reduced the error in surface area from 10-20% down to <5%. To determine the sensitivity of the OpenFOAM results to smoothing, simulations were performed for 'spheres' (actually polyhedra as shown in Figure 9(a)) generated in the HelyxOS graphical user interface and also for voxelized spheres with the same centers and radii, before and after smoothing (Figures 9(c) and 9(d) respectively). Relative to the polyhedral 'spheres', the mean velocity in the flow direction was 7% lower for the voxelized spheres and smoothing reduced this error to 4%. The validation case for a periodically constricted tube shown in Figure 7 was also re-run with a smoothed surface, reducing the mean error from $\pm$2% down to $\pm$1%.

Sub-Grain Scale Model of Seepage

Figure 10 shows the Beads-Cu3 sub-volume, including the boundary conditions applied in the CFD simulation. The pressure gradient of 0.001 kPa across the sub-volume is equivalent to a hydraulic gradient of 0.025; as the resultant Reynolds number <<1 the flow is laminar. As in the validation case, velocity data obtained within about 5 voxels of the input and output boundaries contained some anomolous values. As a result, data within 10 voxels of each boundary were ignored in all subsequent analyses. The 'symmetry' condition used along the side faces enforced a reflection of the velocities near the boundary so that if velocity vectors suggest flow out across the boundary this outward flow is matched by a symmetrical inward flow. This gave no net flow across the side boundaries, but the velocities were not zero along (parallel to) the boundary.

Empirical Validation

Following Narsilio et al. (2009) the hydraulic conductivity values (k_{CFD}) listed on Table 3 were calculated using the applied hydraulic gradient and the velocity component in the flow (Z-) direction, averaged across a perpendicular slice (grey dashed line in Figure 10) . Mass conservation was confirmed as the average velocity values agreed within $\pm$1% considering all the slices in the image. Laboratory permeameter tests were carried out to measure the hydraulic conductivity values (k_{LAB}) for the four materials using samples produced from the same source material and the same preparation techniques. The tests followed the standard procedure (Head, 1994), using a 75mm diameter constant head permeameter, as shown schematically in Figure 4(b) and discussed in Dai (2014). Samples were constructed with a range of densities by varying the number of taps applied to the side

of the cell with a nylon hammer. The samples were then wetted slowly from the base. Full saturation of the samples may not have been achieved using this approach and a subset of additional tests performed where the samples were de-aired by applying a vacuum found no significant effect on hydraulic conductivity. Figure 11 shows that four out of the five CFD results give k_{CFD} values that compare favorably with the laboratory data. The k_{CFD} values were also compared with the commonly used Hazen (1892) empirical formula for cohesionless material', $k = C_H D_{10}^2$ where C_H is an empirically derived constant. C_H values recommended in the literature are typically between 100 and 150, where k and D_{10} have units of cm/s and cm (Carrier, 2003). The Hazen formula is crude, however it is reassuring that the CFD results lie within the range of k values predicted using Equation 1. C_H values back calculated from the CFD results are listed in Table 3 and show no observable pattern with C_u or particle shape, confirming Carrier's (2003) observation that C_H does not have a useful physical significance.

The CFD result for Sand-Cu3[1] is approximately 25% higher than the laboratory range. As noted above, the increased void ratio in Sand-Cu3[1] should result in a higher hydraulic conductivity, but there will always be some discrepancy between permeameter results and measurements in a small sub-volume, due to physical boundary effects such as increased void ratio near the cell wall (Marketos & Bolton, 2010) and incomplete saturation (Head, 2011). The results are all within the range of uncertainty of typical predictive methods, hence the CFD results are deemed to be plausible.

4. OBSERVATIONS OF FLUID FLOW

Flow velocity

Previous studies using CFD simulations on images of granular media (e.g. Narsilio et al. , 2009; Zaretskiy et al., 2010) have highlighted the formation of preferential flow paths within the CFD models and, even within a single void constriction, local velocities can vary significantly. Local pressure and velocity fields, on a representative 2D plane through the 3D simulation of Sand-Cu3[1], are presented in Figure 12.. The head contours shown in Figure 12(a) support the earlier hypothesis; contours are closer together in the vicinity of constrictions, indicating a steeper hydraulic gradient. Due to the conservation of mass, velocities increase significantly in the constrictions where the flow is forced

through a narrower cross sectional area, producing local maxima visible as the lighter shaded areas in Figure 12(b). These local velocity maxima represent the locations where the fluid is most constrained and were defined by Taylor et al. (2016) as 'hydraulic constrictions'.

Many text books (e.g. Harr, 1990; Cedergren, 1989) suggest that the actual velocity in the voids can be approximated by the 'seepage velocity', $v_{seepage} = \frac{v_{discharge}}{n}$, where *n* is the porosity. Figure 13(a) shows discharge and seepage velocities for Sand-Cu3[1], compared against the cumulative distribution of velocities from the CFD simulation (including both velocity magnitude and the component in the flow (Z) direction). Velocity magnitudes normalized by seepage velocity are shown in Figure 13(b) for all five specimens. The seepage velocity crosses the CFD data very close to the median point. However, in all five materials there are velocities 6-8 times larger than the seepage velocity at some locations within the void space. This has important implications in the study of erosion, as some mobile particles will experience velocities 6-8 times higher than the seepage velocity and the drag forces will be higher than those calculated based on the seepage velocity.

Head loss in constrictions

Streamlines have been used in a number of studies on porous rocks (e.g. (Pereira Nunes et al., 2015; Zaretskiy et al., 2010) to identify the paths taken by fluid through the void space. Pereira Nunes et al. (2015) presented a simple method to generate streamlines from 3D velocity vector fields by selecting a start position; following the local velocity vector over a short distance to obtain a new position; then interpolating to find the new velocity vector at this position; and so on to produce a series of points along a streamline, as shown by the grey dots in Figure 12(c). Streamlines are used here to measure the tortuosity, *T* (as described by Bayesteh & Mirghasemi, 2015 and Guo, 2015), and to generate profiles of head loss as fluid flows through the void space. The cumulative distance, *l*, along each streamline is measured, as well as the shortest (straight line) distance from the beginning to end of the streamline, *s*, and T =*l*/*s*. For each specimen 1000 streamlines were generated, starting at a random location near the inflow boundary and continuing until they reached the outflow boundary. Geometric constrictions were defined as 3D planes using the watershed method and the points where streamlines crossed constriction planes were recorded. Figure 14(a) shows head profiles along twenty streamlines, clearly demonstrating that the hydraulic gradient is not constant at the sub-grain-

scale, rather the head-position curve forms a stepped shape. Figure 14(b) shows a single streamline with geometric constrictions marked as crosses, supporting the hypothesis that head losses are significantly larger in the constrictions than elsewhere in the void space.

To quantify the proportion of head loss occurring at constrictions, a rational approach to differentiate flow in the main voids from flow in the constrictions was needed and so the head loss profiles were simplified to a series of linear segments (Figure 14(c)). The hydraulic gradient was measured at each constriction, then the gradient at the mid-point between neighboring constrictions was measured, to give an indication of the hydraulic gradient in the larger parts of the voids. Finally these gradients were extrapolated linearly and their intersections found, forming the grey line in Figure 14(c). While this linearized profile provides a very simple, efficient and repeatable method to partition head loss in constrictions from head loss in voids, it systematically overestimates the head loss at constrictions, producing errors (denoted by ε in Figure 14(c)); typically $\varepsilon/\Delta H_{cons}$ <5%.

The streamlines used in the above analyses do not necessarily pass through the center of constrictions. To address this, and the subjectivity of defining constrictions, an alternative method was also used, based on hydraulic constrictions (local velocity maxima, Figure 12(b)). In this method streamlines started at the velocity maxima and were advanced forwards and backwards a short distance into the voids. The hydraulic gradient representing the larger voids was defined as the point of inflection in the head loss profile, as shown in Figure 14(d). To explain this decision, the hydraulic gradient ($\Delta H/\Delta L$) is steepest at the constriction and it becomes less steep ($\Delta^2 H/\Delta L^2 > 0$) as the void space becomes wider. When the streamline passes the center of the void, it will start to move towards the next constriction and so the hydraulic gradient becomes steeper again ($\Delta^2 H/\Delta L^2$ <0). Hence the center of the void can be defined as the point of inflection, where $\Delta^2 H/\Delta L^2$ changes sign.

Tables 4 & 5 present the relative proportion of head loss in constrictions, quantified using the methods described in Figures 14(c & d), as well as the approximate length of constrictions relative to the wider voids spaces. Table 4 also includes the spacing between constrictions, measured along streamlines and normalized by median particle size (D_{50}). In all specimens, whether full length or local stream lines are considered, approximately 65-75% of the total head loss occurs in the constrictions, even though they account for less than 40% of the total length along streamlines. Analyses using hydraulic

constrictions and short streamlines (Table 5) show similar results for all materials, however streamlines running the full length of the simulation (Table 4) indicate some dependence on material type. Increasing the C_u value from 1.5 to 3 resulted in a noticeable increase (3-7%) in the proportion of head loss in constrictions, while changing from sand to glass beads resulted in a 1–5% increase. These increases in the proportion of head loss at constrictions are due to a combination of two factors: there is an increase in the number of small constrictions as C_u *increases*, as shown in Figure 3; but the dominant factor appears to be a reduction in the spacing between constrictions when C_u increases and also with a change in particle shape (sand to beads), as shown in Table 4. Figure 11 shows a significant difference in the hydraulic conductivity between Sand-Cu3[1] and [2], even though they have very similar CSDs, suggesting that the difference is caused by a small difference in constriction spacing (Table 4). The standard deviations are quite high for all head loss and distance values, indicating that the behavior for a particular constriction or streamline may vary significantly from the average for the whole material.

Analytical models have been used to estimate the spacing between constrictions; an example is shown in Figure 15, with a constriction spacing equal to D_{50}. Wu et al. (2012) propose alternative analytical methods, suggesting constriction spacings less than half of D_{50}. The results in Table 4 suggest that while relatively uniform materials can have constriction spacing close to D_{50}, the spacing reduces for higher C_u values and also reduces for spherical particles relative to sands. None of the values measured were as low as those suggested by Wu et al. (2012), however Wu et al. try to estimate the spacing between soil layers, rather than the distance between constrictions accounting for the tortuosity of flow.

For flow in a pipe, the head loss due to a constriction has long been recognized as the 'Venturi effect' and the magnitude of the head loss is related to the relative size of the constriction as $v_{constric}^2 - v_{pipe}^2 = 2g\Delta H$ (Douglas et al., 1995) . However $v_{constric}.A_{constric} = v_{pipe}.A_{pipe}$ giving

$$\frac{2g\Delta H}{v_{constric}^2} = 1 - \frac{A_{constric}^2}{A_{pipe}^2} \qquad [4]$$

where ΔH is the head loss between pipe and constriction, $v_{constric}$and $v_{pipe}$are the mean velocities across the constriction and the pipe respectively, while $A_{constric}$ and $A_{pipe}$are the corresponding cross sectional areas. For constrictions in sands it is expected that smaller constrictions will produce larger head losses, but the quantitative relationship in Equation 4 cannot easily be applied, both because the geometry of the entry and exit to the constrictions is highly irregular and the fluid crossing the wider parts of the voids will divide amongst a large number of constrictions, hence $v_{constric}.A_{constric} \neq v_{preceding\ void}.A_{preceding\ void}$.

Relating the head loss at a constriction to its size is challenging, because local heterogeneity in the flow can result in two constrictions with the same size, but different orientations, experiencing very different velocities and hence very different head losses. To account for this heterogeneity, Figure 16(a) shows head loss values at each hydraulic constriction in the Sand-Cu3[1] material, normalized by the average velocity across that constriction; the data are plotted against (Constriction diameter)$^{-1}$ as this produces a clearer trend with head loss. The constriction diameter is the diameter of the largest sphere which can pass through the constriction. While there is significant scatter in the data in Figure 16(a), smaller constrictions produce a greater head loss per unit velocity than large constrictions, which agrees with the results of Yazdchi & Luding (2013) and Indraratna et al. (2012) for flow and constriction properties averaged over larger volumes. In Figure 16(a) a linear fit, based on the mean ratio of head/velocity : (Constriction diameter)$^{-1}$, produces a relatively poor r^2 value of 0.5, however quadratic and cubic spline regressions were also attempted and produced r^2 values of only 0.52 and 0.53 respectively. As an alternative, the head losses are plotted in Figure 16(b) based on the left and right sides of Equation 4, where the cross sectional areas were approximated by the square of the distance map values (i.e. the radius of the void space) at the constrictions and at the largest point in the preceding voids. Smaller constrictions (where $1 - A^2_{constric}/A^2_{void}$ tends to 1) produce much higher head losses but, as noted earlier, there is not a clear trend due to the complexity of the void geometry and there is definitely not a linear relationship as suggested by equation 4 for flow in pipes.

Despite the low r^2 values, linear fits for all five materials are presented in Figure 16(c), in terms of the mean and $\pm$1 standard deviation and enable a general overview of the data for all the samples. While results for the glass beads samples are similar, the angular sand particles produce higher head

losses per unit velocity, with the highest head losses in the more uniform Sand-Cu1.5 sample. The specific surface values, *S*, were higher for angular particles than for spheres (shown in Table 3 in terms of $S.G_s$ rather than *S*, to eliminate the effect of differing G_s between sands and glass beads), however these differences were small compared to the difference in hydraulic conductivity (Figure 11). These results indicate that, while the head loss is largely controlled by the size of constrictions, the shape of constrictions (governed by the angularity of the particles) also has an impact on hydraulic conductivity.

5. EVALUATION OF EXISTING MODELS

Kozeny-Carman

The Kozeny-Carmen equation (Carman, 1937) was originally developed to estimate specific surface, *S*, for industrial powders with known hydraulic conductivity, because *S* could not be measured directly (Chapuis & Aubertin, 2003). The equation considers a group of capillary tubes to be an appropriate analogue to the connected void space in a soil, as shown in Figure 1(b). The velocity:head loss relationship for a single tube is given by Poiseuille's law, $v = \frac{\rho_w R^2}{8\,\mu_w}\, i$, where *v* is the average velocity, ρ_w is the fluid density, *R* is the tube radius and μ_w is the dynamic viscosity of the fluid and *i* is the hydraulic gradient. The Kozeny-Carman equation is derived by using geometric properties of the soil to determine a value for *R* to represent the void space. A version of the Kozeny-Carman equation, described by Mitchell & Soga (2005) is given as:

$$k = \left[\frac{1}{k_0}\right] \frac{\gamma_w}{\mu_w} \frac{e^3}{T^2\, S_0^2\, (1+e)} = \left[\frac{1}{k_0\, T^2}\right] \frac{g}{\mu_w\, \rho_w} \frac{e^3}{S^2\, G_S^2\, (1+e)} \qquad [6]$$

where k_0 is an empirical constant, γ_w is the unit weight of the fluid, S_0 is surface area per unit volume and G_s is the specific gravity of the soil. This equation appears to capture the relationship between *k* and void ratio, as well as particle size and gradation (linked to *S*). Some authors have suggested that it is valid for estimating hydraulic conductivity in sands (Carrier, 2003; Chapuis & Aubertin, 2003; Lambe & Whitman, 1969), however this requires values for *S*, *T* and k_0 which cannot be measured. Chapuis & Aubertin (2003) present a simple analytical method to estimate *S* based on the PSD, which assumes spherical particles. Referring to Table 3, $S.G_s$ values estimated using the method by Chapuis & Aubertin (2003) are within $\pm$5% of the values measured from the microCT generated data.

Guo (2015) presents upper and lower bound estimates of T for various porous media, with values of approximately 1.2–1.7 for the porosity range discussed here, while Mitchell & Soga (2005) suggest T values of √2. Referring to Table 3, these estimates of T are not unreasonable.

Mitchell & Soga (2005) suggest k_0=2.5 and Chapuis & Aubertin (2003) suggest combining k_0 and T into an empirical parameter C_{KC}, giving:

$$k = C_{KC} \frac{g}{\mu_w \rho_w} \frac{e^3}{S^2 G_s^2 (1+e)} \quad [5]$$

Backcalculated C_{KC} values are also shown in Table 3: values for the sands are lower than the suggested values of 0.2 (Carrier, 2003; Chapuis & Aubertin, 2003) while 0.2 appears to be a good estimate for the two beads specimens, but there are significant differences between beads and sands. This is evidence that, while the Kozeny-Carman equation can account for particle size, gradation and void ratio, it does not account for particle shape. Back calculated k_0 values are higher than the value of 2.5 suggested by Mitchell & Soga (2005) and there is no clear pattern with C_u or particle shape. As such, it appears that accounting for tortuosity does not improve the accuracy of the Kozeny-Carman equation. These results suggest that if hydraulic conductivity data is available for a particular sand it may be possible to use the Kozeny-Carman equation to account for small changes in PSD or void ratio, but selecting appropriate C_{KC} or k_0 values in the absence of laboratory permeameter data will be extremely challenging.

Indraratna et al. (2012)

Indraratna et al. (2012) estimated constriction sizes analytically for spherical particles in ideal configurations. They compared these CSD estimates with permeameter data for 60 samples of sands and gravels and proposed the following empirical correlation:

$$k_{Indraratna} = 36.91 \, (D_c^m)^{1.644} \quad [7]$$

D_c^m is the mean constriction diameter and values were determined from the CSDs shown in Figure 3. Equation 6 was used to calculate the hydraulic conductivity estimates, $k_{Indraratna}$, given in Table 3. These estimates differ from the CFD results and lab tests by a factor of approximately 2. Given that Equation 7 was based on a large dataset of materials similar to those examined here, the most likely

explanation for this discrepancy is the difference between the CSD measured from images of real specimens and the approximate values used by Indraratna et al. (2012).

6. Conclusions

This paper presents the results of CFD simulations on microCT images of sands and glass beads. The CFD results were validated against permeameter data as well as analytical solutions and are found to agree well, provided that voxelized images are smoothed before generating CFD meshes. 3D datasets of pressures and velocities at the sub-grain-scale were analyzed to determine local velocities and head losses, as well as fluid streamlines, tortuosity and specific surface values, none of which can be accurately measured in the laboratory.

The CFD results show that local velocities at the sub-grain-scale vary significantly from volume-averaged velocity (discharge or seepage velocity), with velocities 6 to 8 times larger than the seepage velocity occurring locally within the void space. This should be taken into account when modelling hydro-mechanical processes including seepage, erosion and contaminant transport. As imaging hardware develops it will be possible to carry out similar studies on a wider range of C_u values but, for the range studied here, the seepage velocity gives a reasonable estimate of the median velocity.

The hypothesis that hydraulic conductivity is governed by void constrictions has been suggested by previous numerical (Yazdchi & Luding, 2013) and empirical (Indraratna et al., 2012) models, but the results presented in the current paper provide a new approach to visualize and quantify the proportion of the head loss which occurs in the constrictions. The main conclusions are:

- Approximately 65-75% of the total head loss occurs at the constrictions, even though the constrictions account for <40% of the total length travelled through the void space.
- An increase in C_u or a change from sand to spherical particles increases the proportion of head loss at constrictions. This appears to be dominated by the spacing between constrictions, rather than changes in the constriction size distribution.
- Five samples (four materials + 1 repeat) with varying particle sizes, gradations, void ratios and particle shapes produce similar relationships between head loss per unit velocity and constriction size.

- While the constriction size governs head loss, constrictions shape (governed by angularity of the particles) has an impact, with larger head losses in angular materials. The irregular shape of constrictions produce much higher head losses than predicted by the Venturi effect for pipes.
- The spacing between constrictions is close do D_{50} for sand with C_u=1.5, but this spacing decreases for higher C_u and for spherical particles.
- Descriptions of void geometry (especially constrictions) are highly subjective and so alternative definitions are considered in this study. The results vary between methods, highlighting that geotechnical engineers using models based on void geometry must consider alternative definitions and determine which is the most appropriate for their model.

The data are used to evaluate previously proposed expressions for hydraulic conductivity, which were developed using grain-scale models. Back calculation of constants from the Kozeny-Carman equation produces values which differ from those in the literature by roughly 30-60%. While the Kozeny-Carman equation accounts for particle size, gradation and void ratio, it does not account for changes in particle shape. The empirical relationship between constriction size and hydraulic conductivity proposed by Indraratna et al. (2012) does not agree with the CFD data.

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