Quantitative Evaluation of Particle Morphology

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Abstract.

In geomechanics research shape is most often qualitatively assessed. Various definitions on how to quantify shape have been applied in the literature. This paper assesses the feasibility of applying these definitions to digital images of sand grains. Firstly the way in which size can be calculated from these digital images is discussed, then the sphericity and convexity definitions proposed by Sympatec (2008) are considered. These definitions of sphericity and convexity (S^{QP}, Cx) are relatively easy to apply. By relating S^{QP} and Cx to the qualitative measures of particle shape that are most often used in geotechnical sample description, we argue that there is significant scope to introduce these measures to engineering practice (Altuhafi et al., 2012). We show that distributions of convexity and sphericity obtained in 2D and 3D analyses differ.

sand; particle size; particle shape

INTRODUCTION

This paper considers the use of image data to quantify particle morphology in a pragmatic way. Firstly the measurement of size is considered, then particle shape. The data considered were obtained from QicPic laser scanning and micro Computed Tomography (μCT). More in-depth analyses of the data can be found in Altuhafi et al. (2012), Fonseca et al. (2012), Cavarretta (2009), Cavarretta et al. (2012) and Fonseca (2011). Both methods are based on particle-scale data. The paper demonstrates that while the image data are often complex, it can be analysed using conceptually simple measures. These measures can be correlated with conventional approaches to quantify particle morphology. Here by examining only particles exceeding 100μm is consideration effectively restricted to sand sized-particles, however subject to the availability of high resolution images these morphological measures could also be applied to silt.

DATA ACQUISITION

QicPic laser scanning

The laser scanning approach (QicPic) uses image analysis (Sympatec, 2008; Witt et al., 2004). In the dry dispersion system used for particles > 100μm, particles fall in a controlled manner along a vertical chute. At the base of the chute they pass between a specially configured light source and a pair of imaging lenses and a camera records a sequence of binary images of the particles. A statistically representative number of particles can be considered in a short span of time. Theoretically, the approach used overcomes the restriction of conventional optical analysis where the particle image plane is orthogonal to the shortest axis of the particle, and so a more realistic measure of true 3D shapes can be attained.

Micro Computed Tomography (μCT)

μCT scans generate three-dimensional images that describe the attenuation of X-rays within the sand samples. As the attenuation is a function of the composition and density of the object and the beam energy, particles and voids can be distinguished. The resultant data allow three-dimensional analysis of particle morphology (e.g. Fonseca et al., 2012a) and fabric (Fonseca et al., 2012b, 2013). A *Nanotom* (phoenix|x-ray, GE) was used to generate the data presented here. In this system the sample was placed between a X-ray source and a detector and rotated step wise 360° around its axis of symmetry. A series of 2D radiographs was obtained, and numerical reconstruction was applied to this image stack to generate the final 3D image using a filtered back projection algorithm (Kak and Slaney, 2001). μCT resolution depends on the sample size and so in the current study sub cores of 5 – 6 mm in diameter were extracted and scanned. The voxel size of most of the images was 5μm, i.e. approximately 0.015 x d_{50}, where d_{50} is the median particle diameter as estimated from the sieve analysis. The sand considered here is Reigate sand, a locked sand that has previously been studied by Cuccovillo and Coop (1997) and Cresswell and Powrie (2004).

After numerical reconstruction, threshold segmentation was applied to differentiate the particle phase and the void space. The individual particles within the particle phase were isolated by applying a morphological watershed algorithm, as proposed by Beucher and Lantuejoul (1979). The output of this process was an image in which the voxels defining a particular particle are assigned an identifying integer value.

PARTICLE SIZE

Traditionally in geomechanics size has been measured using sieve analysis and the sieve aperture size defines particle size. Cavarretta (2009) discusses what is meant by size in the context of irregularly shaped particle when particle-scale data are available. Here the Feret diameters (*F*) were considered, these are the distances between parallel tangents to the particle outline (tangent lines in 2D, tangent planes in 3D). The 2D QicPic images can be analyzed to get minimum and maximum Feret diameters ($F_{min}^{LS}, F_{max}^{LS}$). For the 3D μCT data, principal component analysis (PCA) was applied to determine the major (long), intermediate, and minor axis orientations of each particle. Using this orientation data an orthogonal rotation was applied and each particle was rotated so that its principal axes were parallel to the Cartesian axes. The major (*a*), intermediate (*b*) and minor (*c*) dimensions of the particle were then taken to be $a = \max(x^{rot}) - \min(x^{rot})$, $b = \max(y^{rot}) - \min(y^{rot})$ and $c = \max(z^{rot}) - \min(z^{rot})$, where $\mathbf{x}^{\mathbf{rot}}$, $\mathbf{y}^{\mathbf{rot}}$ and $\mathbf{z}^{\mathbf{rot}}$ are 1D arrays giving the particle's voxel coordinates following rotation. The laser scanning system also gives data for $EQPC^{LS}$, i.e. the diameter of a circle whose area equals the projected area of the particle.

Figure 1(a) compares the particle size distributions for Toyoura sand obtained using these laser scanning measures with sieve analysis and laser diffraction (using a Mastersizer LS100). There are clear differences in the sizes obtained; considering the extreme $d_{50}^{F\max}$ = 325 μm and $d_{50}^{F\min} = 228$ μm. While the sieve data represent a lower bound to the measurements, they are similar to the d^{Fmin} data for the largest 50% (by volume) of particles in the system. The d^{EQPC} values are consistently slightly smaller than the d^{Fmean} values. Altuhafi et al. (2012) considered other sand types and concluded that $d^{F\min}$ is the size measure that most closely corresponds with sieve data. However, the extent of the similarity between the size measures depends on the sand type.

Figure 1(b) compares the particle size distribution data for the reconstituted Reigate sand using μCT data, the QicPic apparatus, and standard sieving. The match between the sieve data and the distribution of *b* values (i.e. intermediate axes lengths) is very good. The maximum and minimum principal axes lengths (*a* and *c*) obtained from the μCT data bound all the data. The F_{max}^{LS} values closely approximate the *a* values, indicating that the QicPic data can correctly identify the maximum particle dimension, but the F_{min}^{LS} values are larger than the *c* values. In this case, the average principal axis length and the $EQPC^{LS}$ values also give a close approximation to the sieve data.

PARTICLE SHAPE

Quantifying particle shape is non-trivial, as discussed by Cavarretta (2009). Typically qualitative measures are used, i.e. , particles are classified as being angular or rounded following Powers (1953) or comparing their particles with the chart provided by Krumbein and Sloss (1963). Digitized image data, such as the 3D data obtained in this study, allow quantitative measurements of particle shape to be made. Here relatively simple size measures are considered. For the laser scanning the aspect ratio is defined as:

$$AR = \frac{d^{F\,min}}{d^{F\,max}}$$

While for the μCT data both the elongation index (*EI=b/a*) and the flatness index (*FI=c/a*) were considered. In 2D the convexity, Cx, is the ratio between the imaged particle area and the area of the convex hull surrounding the particle, while for the 3D μCT dataset Cx is the ratio between the particle volume and the volume of its convex hull.

For the QicPic, sphericity is given by $S^{QP} = \frac{2\sqrt{\pi A}}{P}$ where A is the projected area of the particle, P is the projected perimeter, and $2\sqrt{\pi A}$ is the perimeter of a circle whose area equals the projected particle area. For the μCT data, sphericity calculated as $S = \frac{\sqrt[3]{36\pi V_p^{\;2}}}{SA}$, where V_p is the particle volume and *SA* is the surface area of the particle.

The relevance of these parameters to soil classification can be demonstrated by calculating Cx and S values for the particles in the reference chart proposed by Krumbein and Sloss (1963). Referring to Figure 2, and both Cx and S^{QP} increase with R^{KS} and S^{KS}. As discussed by Altuhafi et al. (2012) no simple relationship between CX and S^{QP} and the Krumbein and Sloss roundness and sphericity measures, S^{KS} and R^{KS} respectively, could be found. However, the meaning of the Cx and S^{QP} values can also be appreciated by reference to Figure 3, which is a plot of representative silhouettes of natural particles for a range of natural sands against their corresponding S^{QP} and Cx values. The figure also indicates that those particles with higher Cx and S^{QP} are more rounded and spherical.

Altuhafi et al. (2012) presented a database of Cx, AR and S^{QP} values for 36 different sands that have been used in laboratory research. Many of these sands are considered reference sands and qualitative descriptions of their shape were found in a literature review. This literature revealed that the use of a qualitative classification can lead to disagreement, e.g. Fontainebleau sand has been described as angular, subangular, subrounded and rounded and the Toyoura sand has been considered rounded, subangular and subrounded by different researchers. Figure 4 presents median values of sphericity and convexity for the 36 sands and demonstrates that it is possible to empirically correlate these measures with qualitative shape descriptors.

Figure 5 compares the convexity and sphericity values for the Reigate sand that were obtained from laser scanning and μCT . The QicPic images had a pixel size of 10 microns compared to the voxel size of 5 microns used in the CT images. The 3D convexity values tend to be lower than the 2D values, while the 3D sphericity values tend to exceed the 2D values. In both cases the range or distribution of values is markedly higher for the 3D data.

CONCLUSIONS

Image based quantification of particle morphology is now possible. While complex analytical tools can be applied to these images (e.g. Fourier descriptor analysis, Bowman and Soga, 2001), alternative, conceptually simple size measures can be used. Considering particle size, there is not a simple relationship between the image-based measures and sieve data. For many sands, if 2D laser scanning data are considered, the Feret minimum diameter gives a good appropriation to sieve data, however there are exceptions to this (e.g. the Reigate sand considered here). Sphericity and convexity can be related to well-established quantitative and qualitative measures of particle size. While equivalent definitions of sphericity and convexity can be applied to 2D and 3D values, the values calculated and their distribution will differ. More detailed analyses of the datasets considered here are given in Altuhafi et al. (2012) and Fonseca et al. (2012).

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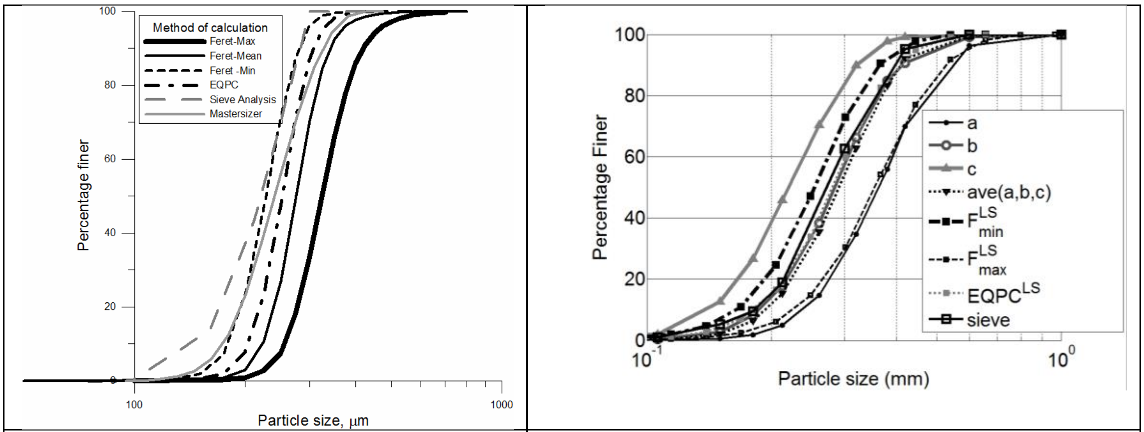


(a) Toyoura Sand | (b) Reconstituted Reigate Sand

Fig. 1. Representative particle size distributions obtained from image based analysis

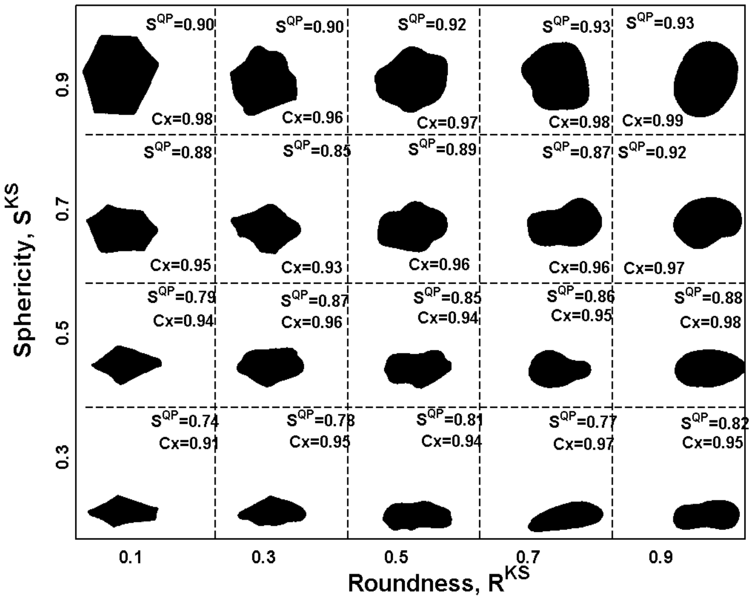


Fig. 2. 2D sphericity and convexity values for the reference chart proposed by Krumbein and Sloss (1963)

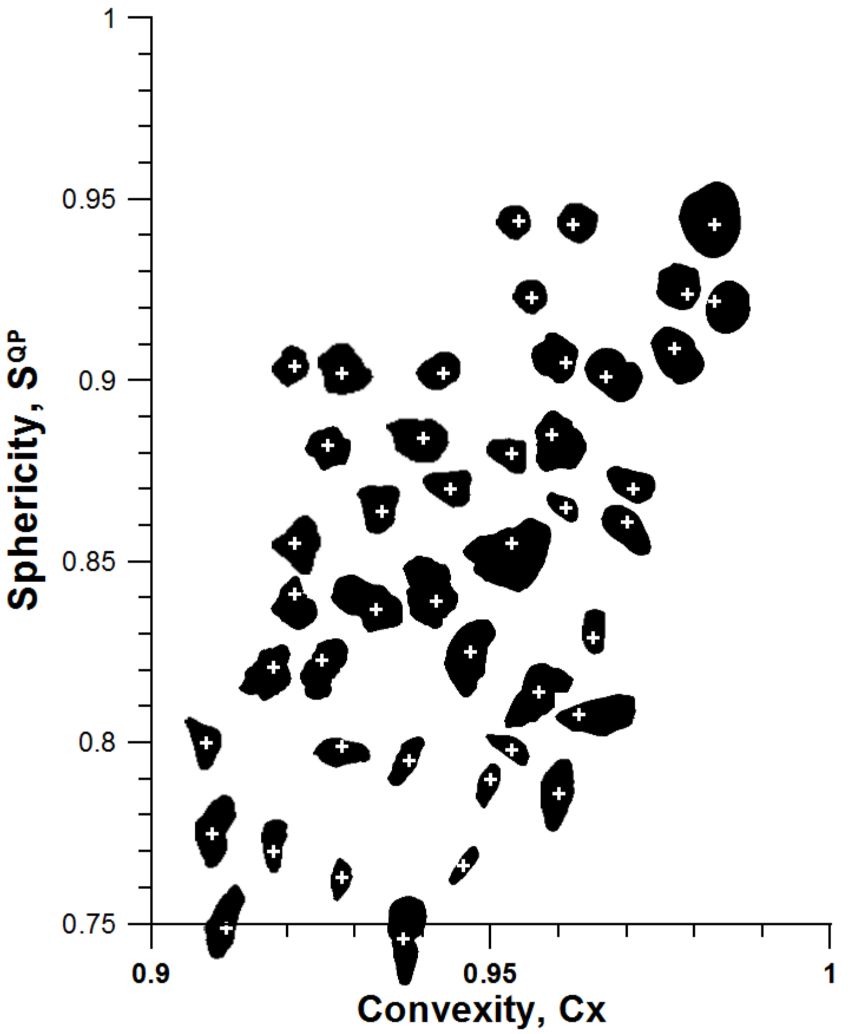


Fig. 3. Representative sand grains plotted against their S^{QP} and Cx values.

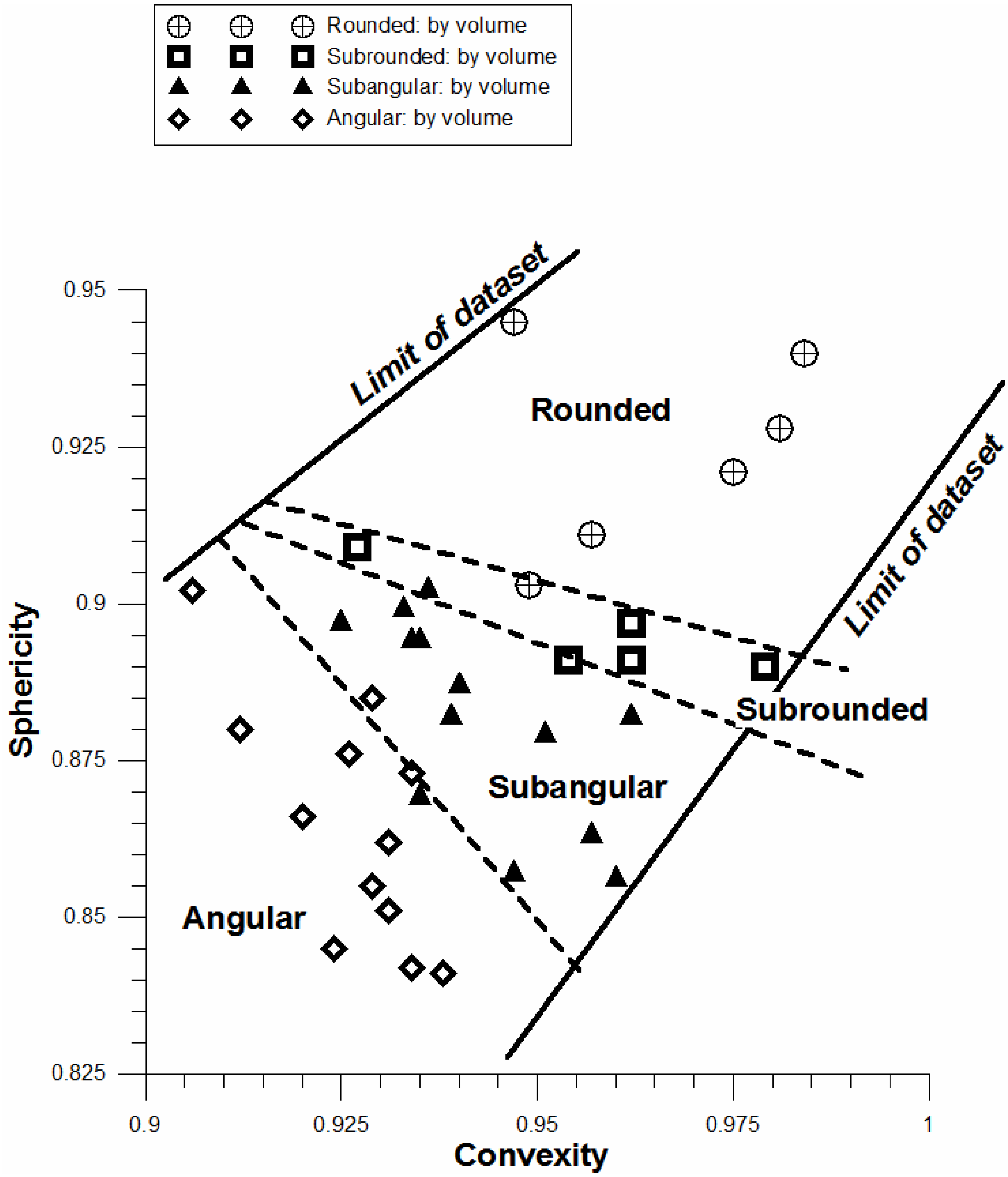
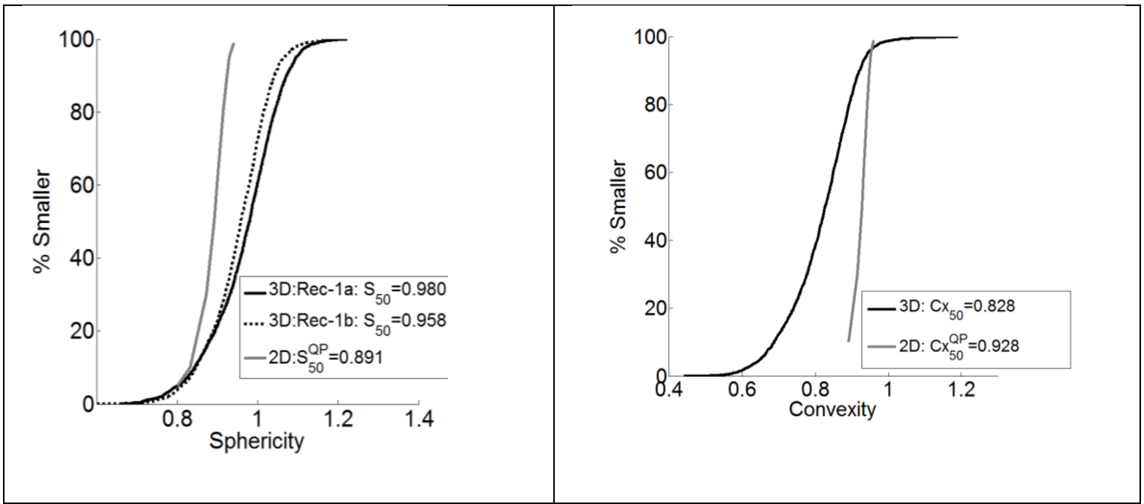


Fig. 4. Correlation between S^{QP} , Cx values and qualitative descriptions of sand particles.



(a)	(b)

Figure 5: Comparisons of 2D and 3D measures of sphericity and convexity for Reigate sand.