Computers and Geotechnics 78 (2016) 11–24

Contents lists available at ScienceDirect

Computers and Geotechnics

journal homepage: www.elsevier.com/locate/compgeo

Research Paper

The fractal micro mechanics of normal compression

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ARTICLE INFO

Article history:
Received 18 January 2016
Received in revised form 6 April 2016
Accepted 29 April 2016

Keywords:
DEM
Normal compression
Crushing
Fractal

ABSTRACT

The fundamental fractal micro mechanics of normal compression of granular materials is studied using DEM. This paper examines the emergence of a finite fractal bounded by two particle sizes as stress increases, and the evolution of various definitions of the 'smallest particles'. It is revealed that if particles are categorised according to their coordination number, then the volume of all particles with 4 contacts or fewer is directly proportional to the void space. These particles are called 'critical particles' and are shown, for the first time, to explain quantitatively the voids reduction with increasing vertical stress.

1. Introduction

The authors have recently published much work accurately modelling the one-dimensional and isotropic normal compression of sand using the discrete element method [1–3]. The most notable outcome of this work was the development of a new compression law, in which the slope of the normal compression line (NCL) is solely a function of the size-hardening effect of the individual particles. The NCL is linear when plotted on two logarithmic axes, and the compression law is given by:

$$\log e = \log e_y - \frac{1}{2b}\log\frac{\sigma}{\sigma_y} \tag{1}$$

where e is the current voids ratio, e_y is the voids ratio at yield, σ is the current stress, σ_y the stress at yield, and $1/2b$ describes the slope of the compression line, where b represents the size effect on particle strength σ_{av}:

$$\sigma_{av} \propto d^{-b} \tag{2}$$

where d is particle size (diameter). The basis of the above compression law is that a fractal particle size distribution (PSD) emerges as a result of particle crushing during normal compression. It was shown in the authors' previous work, by analysing the distribution of particles and contacts that fractal PSDs do indeed emerge during compression [1]. The first aim of this paper is to provide an in-depth analysis of the development of a fractal particle size distribution produced by particle crushing, and in particular what occurs at the fine end of such a distribution as new particle sizes emerge. The second is to examine some of the assumptions in and validate the compression law given in Eq. (1), and to quantitatively ascertain which particles determine the current voids ratio.

2. Background to model

The work presented here uses a cylindrical sample, initially 20 mm × 20 mm in size, subjected to one-dimensional normal compression to a stress of 45 MPa. The initial sample consists of 857 spheres, 2 mm in diameter, enclosed within rigid walls. The particles are attributed strengths in terms of octahedral shear stress, q:

$$q = \frac{1}{3}\left[(\sigma_1-\sigma_2)^2+(\sigma_2-\sigma_3)^2+(\sigma_1-\sigma_3)^2\right]^{1/2} \tag{3}$$

where σ_{1-3} are the average principal stresses within the particle, which are returned by the discrete element software, PFC3D 5 [4]. This breakage criterion was chosen as it provides a convenient measure of particle stress, that can be applied to the case of diametral compression (for which the available particle strength data relates to), while also being able to take into account more complex loading geometries, with multiple contacts. The use of Eq. (2) means that a particle loaded with few contacts will, in general, have a larger stress than one loaded more uniformly with many contacts, and therefore would be more likely to break, which seemed physically reasonable. Fundamentally, this criterion satisfies the requirements of taking into account multiple contacts and leads to the correct normal compression behaviour (i.e. the correct slope of the NCL and fractal particle size distributions [1]).

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http://dx.doi.org/10.1016/j.compgeo.2016.04.018
0266-352X/

The strengths are attributed to the particles according to a Weibull distribution, where the modulus, m, is 3.3 and the characteristic strength, q_0 is a function of particle size according to:

$$q_0 \propto d^{-3/m} \tag{4}$$

The characteristic strength, q_0, is a value of strength such that 37% of particles are stronger, and is used as a gauge of the average strength for a particular particle size (it is similar in magnitude and proportional to the mean value of the distribution). Weibull statistics are commonly applied to soil particle fracture [e.g. 5,6], a justification of which can be found in McDowell and Amon [7]. The modelling procedure and breakage mechanism is identical to that used in all of the previous works by the authors' [e.g. 1]. The modulus of 3.3 is obtained from experimental particle crushing tests [8], as are the strengths.

When a particle breaks, it is replaced by two smaller sphere fragments, equal in size to one another, and which together have the same volume as the original sphere, ensuring conservation of mass. Particles always split into 2 fragments, and the size ratio of any new fragment and its 'parent' sphere is constant, regardless of scale. The new fragments overlap to an extent that they are located within the boundary of the original sphere (shown schematically in [1,2,9]). The two new fragments are aligned in the direction of the minor principal stress axis of the breaking 'parent' particle. Although this overlap causes an increase in local pressure, the two fragments move apart in the direction of the minor principal stress, just as would occur for a single particle crushed between flat platens. Particle breakage is implemented by checking all particles at once, and all particles in which the stress is greater than the strength are replaced by fragments. The overlap between new fragments is released immediately upon breakage by completing a number of computational timesteps, during which time the particles are allowed to move apart until the system is stable and has reached equilibrium. In previous work [1], the use of 3 and 4 fragments in a symmetric splitting mechanism was also investigated, and it was found that there were no differences in either the normal compression lines or the ultimate particle size distributions. In additionally, using random, non-symmetrical fragmentation mechanisms (following experimental observations) also results in no differences to the resulting NCL or PSDs.

The sequential modelling procedure begins by applying a macroscopic stress increment to the sample. Particles are then checked and allowed to break if necessary. If any particles break, they are replaced by fragments, which are then allowed to move apart, releasing the energy induced by the artificial overlap. This continues until no further breakages occur, after which the macroscopic stress is *re*-applied. Once a macroscopic stress is achieved with no subsequent breakage, the simulation continues and the next stress increment is applied. This continues until the simulation reaches a point where the size of the smallest particle renders the timestep too small to be computationally economical, which is at 45 MPa in the simulation presented here.

The macroscopic stress increment used is 125 kPa, and maximum velocity of the upper boundary is limited at 0.1 m/s. Gravity is not applied in these simulations. The voids ratio is calculated using the volume of particles and the volume of the container, and is calculated after the overlap and artificial energy has been dissipated following breakages. Relevant model specifics are given in Table 1, however, for full details on the modelling procedure, including discussion of its limitations, the use of the octahedral shear stress as a criterion, the breakage mechanism, and how the principal stresses are calculated, readers are directed to prior publications [1,2,10].

Table 1
Summary of DEM properties for the simulation.

General simulation properties	
Oedometer size: height × diameter (mm)	20 × 20
Contact model	Hertz–Mindlin
Wall friction coefficient	0
Wall shear modulus, G (GPa)	75
Wall Poisson's ratio, v	0.30
Particle friction coefficient	0.5
Particle shear modulus, G (GPa)	28
Particle Poisson's ratio, v	0.25
Particle density (kg/m^3)	2650
Initial (largest) particle size, d_1 (mm)	2
Initial no. of particles	857
Initial voids ratio	0.75
Initial particles (d_1) 37% strength (MPa)	37.5
Weibull modulus, m	3.3
Final no. of particles	25,527
Final voids ratio	0.43

3. Normal compression results

The DEM normal compression results are given in Fig. 1, along with experimental results for the sand that the strength data is obtained from. The slope of the compression line according to Eqs. (1) and (3) should be approximately 0.5, this ideal slope is shown in the figure by the dashed line. As can be seen, the simulation, as well as the experimental results demonstrates agreement with the slope predicted from the size-hardening law for the particles. The simulation is also consistent with the authors' previous results using the same particle properties (although the current work uses a statistically different sample, of a different shape). The yield stress σ_y is approximately 10 MPa.

Progressive particle size distributions from the simulation are shown in Fig. 2(a), at 5 MPa intervals. The PSDs are shown in the conventional manner: the percentage by mass finer plotted against particle size, on semi-logarithmic axes. To avoid clutter, only the extreme PSDs are labelled in the figure, i.e. at 5 MPa and 45 MPa, the intermediate curves are in consecutive order. Experimental PSDs for the corresponding silica sand are given in Fig. 2(b). The use of a monodisperse initial sample in the simulation allows the

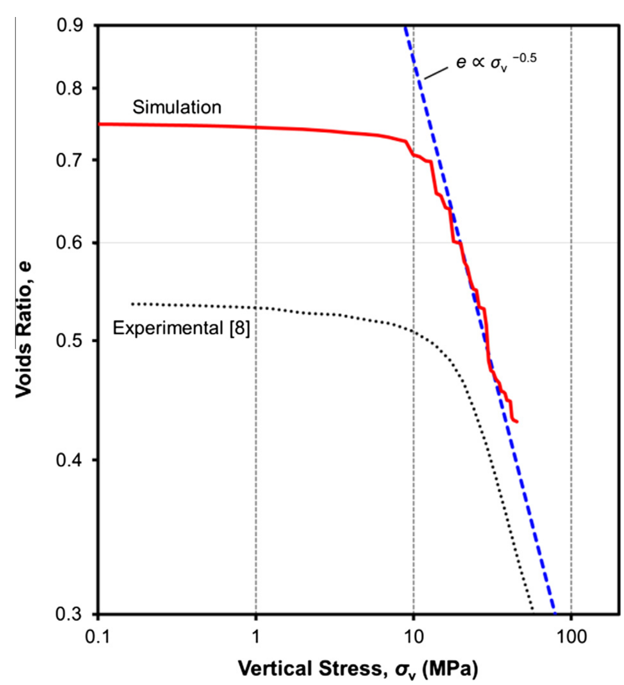

Fig. 1. Normal compression behaviour for simulation of crushable sand.