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SCALING OF DISCRETE ELEMENT MODEL PARAMETERS IN UNIAXIAL TEST SIMULATION

Subhash C Thakur[+,*], Hossein Ahmadian[+], Jin Sun[*], and Jin Y. Ooi[*]

** School of Engineering, University of Edinburgh,*

King's Buildings, Edinburgh EH9 3JL, UK

+ Newcastle Innovation Centre, Procter and Gamble Technical Centre Ltd, Newcastle upon Tyne, NE12 9BZ, UK.

This study investigates the scaling of DEM model parameters that are necessary to produce scale independent predictions for cohesionless and cohesive solid under confined compression and unconfined compression to failure. A bilinear elasto-plastic adhesive frictional contact model was used[1]. The results show that contact stiffness (both normal and tangential) for loading and unloading scales linearly with the particle size and the adhesive force scales very well with the square of the particle size. This scaling law would allow scaled up particle DEM model to exhibit bulk mechanical loading response in uniaxial test that is similar to a material comprised of much smaller particles. This is a first step towards a mesoscopic representation of a cohesive powder that is phenomenological based to produce the key bulk characteristics of a cohesive solid and has the potential to gain considerable computational advantage for large scale DEM simulations.

INTRODUCTION

The discrete element modelling originally developed by Cundall and Strack[2] has increasingly been used to model many problems involving discrete phenomena including powder packing compaction, powder flow, rotating drum, mixing, hopper flow, fluidized bed, pneumatic conveying and so on. A detailed report on the application of DEM can be found in the paper by Zhu et al. [3]. The DEM simulations of the aforementioned phenomena have given many significant insights into the microscopic details at particle level and useful information to understand complex behaviour exhibited by granular material. For fine particles, the biggest shortcomings of DEM simulations for practical applications are the challenge of modelling very small particles and the lack of computational power. Even the smallest industrial processes involve interaction of trillions of particles, and it becomes computationally impossible and impractical to account for every individual realistic size particles.

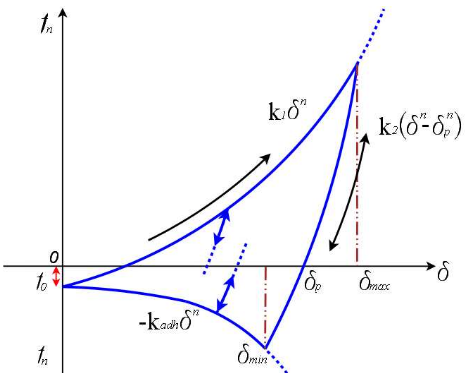
There can be several possible solutions[4] for the speed-up of DEM simulation, such as *optimization of the hardware and the software, including improving DEM algorithm, parallel computing, and simplifying the calculation process*. One common way is to *simplify the calculation process,* for example, using a lower spring stiffness, using mono-sized particles, using a cut-off distance for long range forces[4] etc. Other possibilities are the use of higher particle density in quasi-static simulation[5] (density scaling), reduction of number of particles by scaling the system size down or scaling up the size of particle. Poschel et al[6] proposed a general approach to scale down the experiments to laboratory size. They found that the dynamics of their granular system changed if all sizes were scaled by a constant factor, but leaving the material properties the same.

Such kind of approach is more suitable for problems in geo-mechanics where original physical problem is scaled down to a laboratory model to get the same results. Another scaling approach is to use larger size elements (particles) to reduce the number of particles whilst keeping the original system size the same. This approach is sometimes referred to as coarse graining approach and has been used by a few researchers in the field of cavity filling[7], pneumatic conveying[8], and rotary drum[9]. In this approach, DEM parameters are adjusted such that DEM simulation result exhibits the same dynamic and static properties as the experimental granular material.

In this study, an attempt was made to investigate the scaling of contact stiffness (normal and tangential) and adhesive force in the cohesive contact model that would permit a mesoscopic representation of a cohesive powder using much larger DEM particles. The target is for the DEM model with scaled up particle to exhibit the compression and shearing bulk behaviour in a uniaxial test exhibited by a cohesive powder.

DEM CONTACT MODEL

DEM contact model based on the physical phenomena observed in adhesive contact experiments has been proposed [10]. When two particles or agglomerates are pressed together, they undergo elastic and plastic deformations and the pull-off (adhesive) force increases with an increase of the plastic contact area. A non-linear contact model that accounts for both the elastic-plastic contact deformation and the contact-area dependent adhesion is proposed. The schematic diagram of normal force-overlap (f_{ep}– δ) for this model is shown in Figure 1.



$$f_{hys} = \begin{cases} k_1\delta^n & \text{if } k_2\,(\delta^n-\delta_p^n) \geq k_1\delta^n \\ k_2\,(\delta^n-\delta_p^n) & \text{if } k_1\delta^n > k_2\,(\delta^n-\delta_p^n) > -k_{adh}\delta^n \\ -k_{adh}\delta^n & \text{if } -k_{adh}\delta^n \geq k_2\,(\delta^n-\delta_p^n) \end{cases} \quad (1)$$

Where: k_1 = the virgin loading stiffness parameter,
k_2 = the unloading/reloading stiffness parameter,
k_{adh} = the adhesive stiffness parameter
n = the non-linear index parameter

Fig 1. – Normal contact force-displacement function for the implemented model.

As a first step towards scaling of DEM model parameter, a simplified linear version of the contact model (parameter n=1)[11,12] with K_{adh}=0 is explored (see Fig. 2a). The model was used to simulate uniaxial confined and unconfined loading of cohesionless and cohesive powder.

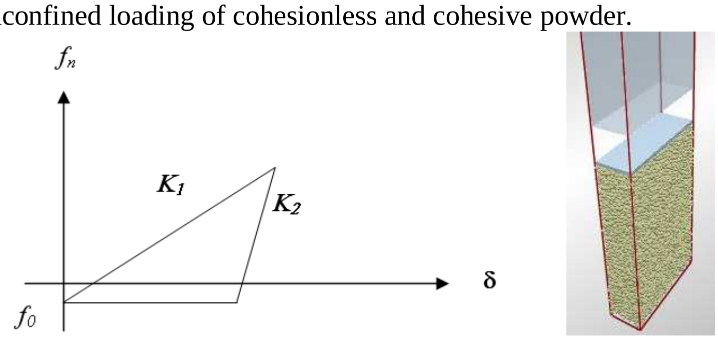


Fig 2. a) Simplified contact model and b) simulation set up

For cohesionless system the contact loading and unloading stiffness is scaled ***linearly*** with the radius. And for a cohesive system, ***linear, quadratic, and cubic scaling*** of adhesive forces with particle radius is investigated. The theoretical background behind these scaling laws will be presented elsewhere.

SIMULATION SET-UP

The computer simulations reported here consider a series of uniaxial compression tests in a rectangular cuboid (see Fig. 2b) of 50 mm thickness (>5*diameter of largest particle), 150 mm width, and 300 mm height. Periodic boundaries were used along X and Y direction to avoid the wall effect. The cuboid contains a top and a bottom plate. A series of uniaxial compression simulations were conducted using the simplified DEM contact model. Each simulation consisted of several stages of loading: a) filling the cuboid (and compressing the assembly to 5kPa which provided an initial packing at a relatively low stress level for cohesive system); b) confined consolidation to a much higher stress level and subsequent unloading, c) and finally unconfined compression of the sample to failure after the removal of the confining mould.

Compression was achieved by moving the top plate at a constant speed until a desired bulk vertical stress was attained. Subsequently, unloading was performed by an upward retreat of the upper plate. The confining periodic boundaries were then removed and the unconfined samples were allowed to reach the new equilibrium, and finally the top platen was lowered to fail the sample. The loading and unloading were performed at an axial speed of 10 mm/s (strain rate<$0.05s^{-1}$) throughout = to ensure quasi-static loading. The lower plate remains stationary in all stages.

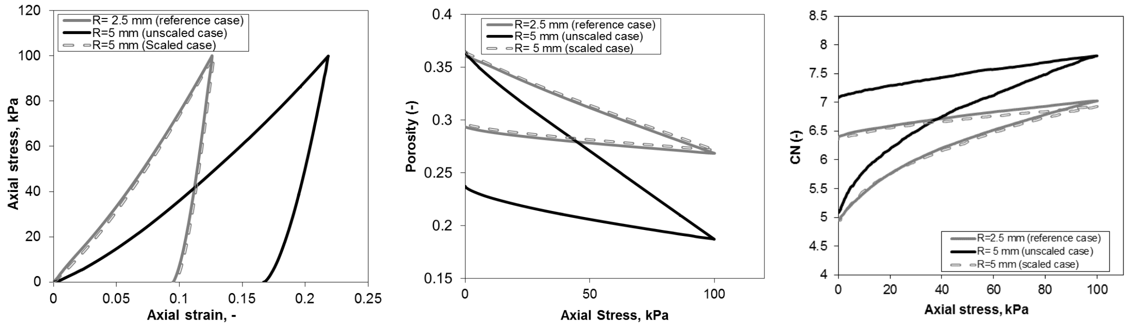
The scaling law was first explored for the cohesionless case and then for the constant adhesion case. The parameters used in the simulations are listed in Table 1. The particle shape used in this study was spherical and uniform size. The cohesive contact model was only applied to particle-particle interactions. The particle-geometry interactions were modelled using the Hertz-Mindlin (no-slip) contact model and hence no particle-geometry adhesion was included.

Particle Density, ρ (kg/m³)	*2000*
Loading Spring Stiffness, K_1 (N/m)	$5x10^3$ to $1x10^4$
Unloading Spring Stiffness, K_2 (N/m)	$2.5x10^4$ to $5x10^4$
Adhesion force, f_0 (N)	0 to -1.6
Tangential Stiffness, K_t (N/m)	2/7 K_1
Particle Static Friction, μ_{sf}	0.5
Particle Rolling Friction, μ_{rf}	0.001
Particle radius (R), mm	2.5 to 5
Top and bottom platen Friction, μ_{Pf}	0.3
Simulation Time step (s)	$1x10^{-5}$

Table 1. Input parameters

SIMULATION RESULTS

Cohesionless System. The axial stress vs axial strain and the coressponding stress-porosity behaviour during the confined loading and unloading simulation are shown in Figures 3a and 3b respectively. The simulation with 2.5 mm (R=2.5 mm) particle is taken as the reference case. The particle density and sample porosity were kept the same throughout to keep the density of gravitational potential energy the same in both the large particle and the small particle systems. For the first case (unscaled), the particle size was increased to 5mm without scaling the stiffness (all model parameters unchanged). It can be clearly seen that increasing the particle size without scaling the stiffness produces a softer bulk response compared to the reference case. However, when stiffness was scaled linearly with the particle radius, the stress-strain response and the corresponding porosity-stress response for the 5mm particle converged to that for the reference case of 2.5mm particle. It can be concluded that the same bulk loading and unloading stiffnesses are predicted for the simulations with scaled contact normal and tangential stiffness. However, there was a discrepancy when particle size was increased without scaling the stiffnesses.

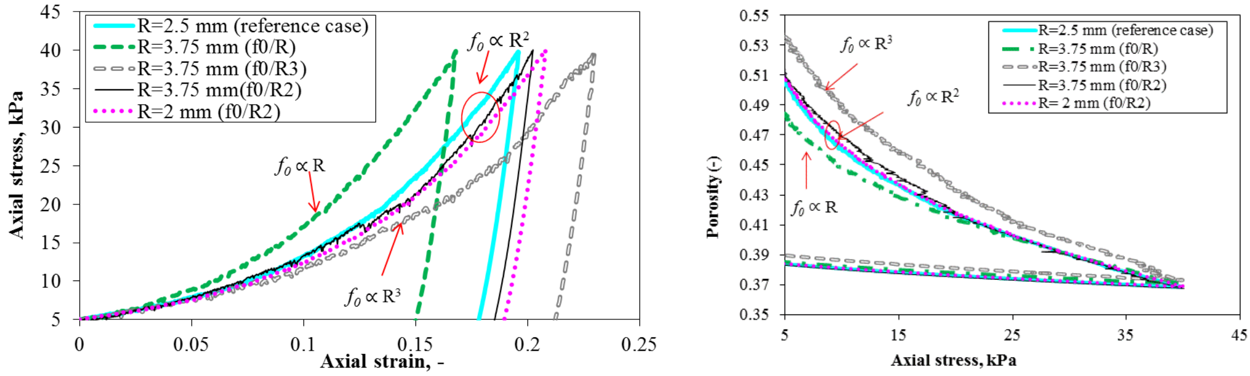


(a) (b) (c)

Fig 3. a) Axial stress vs axial strain b) Axial stress vs. porosity in uniaxial compression test c) Evolution of CN during uniaxial test

An investigation of the coordination number (CN) in the systems is shown in Figure 3c. This shows that the CN during the loading and unloading also evolved in the same fashion for the reference case and the scaled simulation, however, the CN for the unscaled case increased at a higher rate compared to the reference case.

Cohesive System. For the cohesive system, the normal and tangential stiffness (both loading and unloading) were scaled linearly as in the cohesionless system. Additionally, linear, quadratic, and cubic scaling of the adhesive force parameter f_o with particle radius was explored. The simulation with particle size of 2.5 mm was the reference case. The axial stress vs strain and the corresponding porosity-stress response are shown in Figures 4a and 4b respectively for different particle sizes with different scaling approaches for the adhesive force. When the adhesive force was scaled linearly with particle size, the initial porosity at 5kPa stress level (Fig 4b) was found to be lower when compared to the quadratic and cubic scaling (denoted by **-**). The linear scaling produced less compression under loading than the quadratic and cubic scaling as shown in stress-strain curve (Fig 4a). Conversely the cubic scaling of adhesive force with particle size produced a higher initial porosity and the sample compressed the most during loading The quadratic scaling of adhesive force with particle size produced very similar stress-porosity and stress-strain response for particle size in a range of 2 to 3.75 mm.



(a) (b)

Fig 4. a) Axial stress vs strain; b) Axial stress vs porosity in confined compression

Note: The letters in parenthesis indicates the degree of scaling with radius.

The scaling of the adhesive force was further examined by looking into the unconfined compression behavior. As shown in Figure 5, the quadratic scaling produced very similar unconfined stress-strain behaviour to shear failure for different size particles of 2-3.75mm. However, the linear scaling with particle size underestimated the unconfined strength and cubic scaling overestimated the strength.

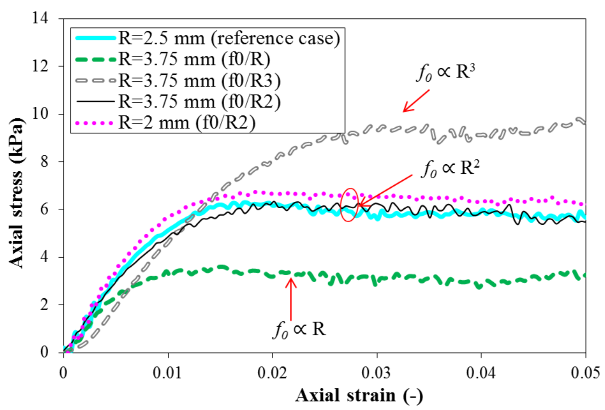


Fig 5. Uniaxial compression to shearing of the sample

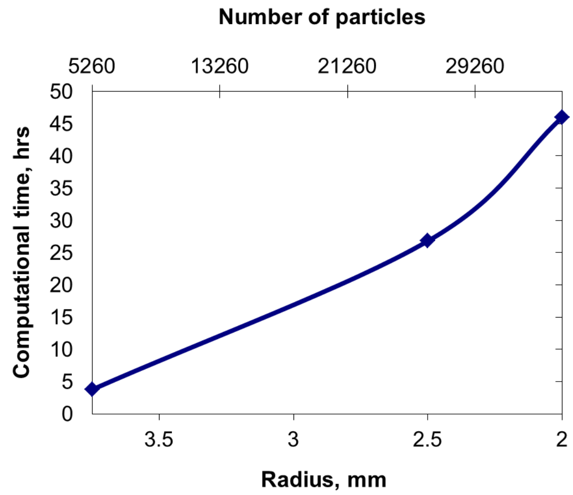


Fig 6. Computational time reduction

The above analysis has clearly shown that that adhesive force scales quadratically with the particle radius. This is consistent with findings from Rumpf[13] that quadratic scaling of adhesive force with particle size keep tensile strength of bulk powder approximately constant as the DEM particles vary in size. The combined linear scaling of the spring contact stiffness and quadratic scaling of the adhesive force parameter appear to be a robust strategy for the upscaling of particle size. This is consistent with results from Walton and Johnson [9] on the DEM simulations of rotary drum flows using their previously implemented DEM code [14]. They found that the scaling of the pull-off force with the square of the particle size produced flows that were qualitatively in agreement.

The scaling laws allow the use of larger particle sizes whilst reproducing similar mechanical response of a particulate assembly with smaller particles and help to reduce the computational time significantly. Figure 6 shows a nine fold decrease in computational time if particle size is scaled from 2mm to 3.75mm for the simulation of uniaxial compression using 12 core processors in this study.

CONCLUSION

A study of the scaling laws to produce scale independent computations of confined compression and unconfined loading has been presented. In the linear spring model with elasto-plastic deformation and no cohesion, the contact loading and unloading stiffness (normal and tangential) scales linearly with particle size. A very good agreement in the macroscopic (stress-strain and stress-porosity relations) and the microscopic (stress-coordination number relation) behaviour was found for different particle sizes when the contact stiffness was scaled linearly. For the simulation with a constant adhesion, the scaling of the adhesion force parameter with the square of the particle radius (2~5mm) produced confined stress-strain and stress-porosity behaviour, and unconfined stress-strain behaviour that remained remarkably similar as the size of the particles were increased. Thus, by scaling the stiffness linearly and adhesive force quadratically, a DEM model using larger particle size can exhibit the same bulk properties as the system with small particle size. The scaling may break down for effects that intrinsically depend on grain size. Nevertheless, such scaling laws are particularly useful for studying very large scale particulate systems with considerably less computational time.

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