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Scaling of discrete element model parameters for cohesionless and cohesive solid

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ABSTRACT

One of the major shortcomings of discrete element modelling (DEM) is the computational cost required when the number of particles is huge, especially for fine powders and/or industry scale simulations. This study investigates the scaling of model parameters that is necessary to produce scale independent predictions for cohesionless and cohesive solid under quasi-static simulation of confined compression and unconfined compression to failure in uniaxial test. A bilinear elasto-plastic adhesive frictional contact model was used. 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 a 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 industry scale DEM simulations.

1. Introduction

The discrete element modelling originally developed by Cundall and Strack [3] has increasingly been used to model many problems involving discrete phenomena including powder packing [21,35], compaction [14,26], powder flow [19,27–29], rotating drum [33], mixing [2], hopper flow [8,12], fluidized bed [34], pneumatic conveying [6,25] and many others. A detailed report on the applications of DEM can be found in the review paper by Zhu et al. [36]. 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, one major shortcoming of DEM simulations for practical applications is the challenge of modelling very small particles. Even the smallest industrial processes involve interaction of trillions of fine particles, and it becomes computationally impossible and impractical to account for every individual realistically sized particles.

There are several possible solutions [18] for the speed-up of DEM simulation, such as optimization of the hardware and the software, including improved DEM algorithm, parallel computing, and simplifying the calculation process. Common ways to simplify the calculation process are done, for example, using a lower spring stiffness, using mono-sized particles, and using a cut-off distance for long range forces [18]. Other possibilities are the use of higher particle density in quasi-static simulation [26] known as density scaling, reduction of number of particles by scaling the system size down or scaling up the size of particle. Pöschel et al. [22] 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.

Pöschel's approach is more suitable for problems where an original physical problem is scaled down to a laboratory model in an attempt to obtain a physical model of the problem. This approach may not reduce the computational time in DEM modelling because the number of particles still remains the same and the particle size is also reduced. One possible solution is to use larger size elements (particles) to reduce the number of particles whilst keeping the original system size the same, however, this would violate geometric similarity and may introduce some error in the bulk response as reported in Feng et al. [7]. The major issue in this kind of approach is to adjust DEM model parameters such that large particle DEM simulation result exhibits the same dynamic and static properties as small size realistic particles. This approach is sometimes referred to as coarse graining approach and has been used by a few researchers in the field of cavity filling [1], pneumatic conveying [25], and rotary drum [33].

This study investigates the scaling of model parameters that is necessary to produce scale independent predictions for cohesionless and cohesive powder under quasi-static 3D simulation of confined compression and unconfined compression to failure. The target is to develop

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DEM model with scaled up DEM particle to exhibit the compression and shearing bulk behaviour in a uniaxial test exhibited by powders.

2. DEM model and theoretical background for scaling

2.1. DEM contact model

A DEM contact model based on the physical phenomena observed in adhesive contact experiments has been proposed [11]. 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. Fig. 1 shows the contact model in its full generic form which captures the key elements of the frictional-adhesive contact mechanics in that: f_0 provides the van der Waals type pull-off forces; k_1 and k_2 provide the elasto-plastic contact; k_{adh} provides the load dependent adhesion; the exponent n provides the nonlinearity and the resulting contact plasticity defines the total contact adhesion. The model is thus expected to be capable of modelling fine powders to study phenomena such as agglomeration, attrition and flow.

The schematic diagram of normal force–overlap (f_n–δ) for this model is shown in Fig. 1. When n = 1 the model becomes linear (Fig. 1b) and similar to existing contact models [14,32,37]. The linear version of the contact model is used in this study. The details of the contact model are presented elsewhere [28,29].

This contact model has been implemented through the API in EDEM® v2.3, a commercial DEM code developed by DEM Solutions Ltd. [4]. The total contact normal force, f_n, is the sum of the hysteretic spring force, f_{hys}, and the normal damping force, f_{nd}:

$$f_n = \left(f_{hys} + f_{nd}\right)\boldsymbol{u}, \tag{1}$$

where, $\boldsymbol{u}$ is the unit normal vector pointing from the contact point to the particle centre. The force–overlap relationship for normal contact, f_{hys}, is mathematically expressed by Eq. (2).

$$f_{hys} = \begin{cases} f_0 + k_1\delta^n & \text{if } k_2\left(\delta^n - \delta_p^n\right) \geq k_1\delta^n \\ f_0 + k_2\left(\delta^n - \delta_p^n\right) & \text{if } k_1\delta^n > k_2\left(\delta^n - \delta_p^n\right) > -k_{adh}\delta^n \\ f_0 - k_{adh}\delta^n & \text{if } -k_{adh}\delta^n \geq k_2\left(\delta^n - \delta_p^n\right) \end{cases}. \tag{2}$$

The normal damping force, f_{nd}, is given by:

$$f_{nd} = \beta_n v_n \tag{3}$$

where v_n is the magnitude of the relative normal velocity, and β_n is the normal dashpot co-efficient expressed as:

$$\beta_n = \sqrt{\frac{4m^* k_1}{1 + \left(\frac{\pi}{\ln e}\right)^2}} \tag{4}$$

with the equivalent mass of the particles m^* defined as $(m_i m_j / m_i + m_j)$, where m is the mass of the respective particles, and the coefficient of restitution e defined in the simulation.

The contact tangential force, f_t, is given by the sum of tangential spring force, f_{ts}, and tangential damping force, f_{td}, as given by:

$$f_t = (f_{ts} + f_{td}). \tag{5}$$

The tangential spring force is expressed in incremental terms:

$$f_{ts} = f_{ts(n-1)} + \Delta f_{ts}, \tag{6}$$

where $f_{ts(n-1)}$ is the tangential spring force at the previous time step, and Δf_{ts} is the increment of the tangential force and is given by:

$$\Delta f_{ts} = -k_t \delta_t, \tag{7}$$

where k_t is the tangential stiffness, and δ_t is the increment of the tangential displacement. Whilst varying values for the tangential stiffness have been used in the literature, in this study it is set as $2/7k_1$ [31]. The tangential damping force is product of tangential dashpot coefficient, β_t, and the relative tangential velocity, v_t, as given by Eq. (8):

$$f_{td} = -\beta_t v_t. \tag{8}$$

The dashpot coefficient β_t is given by:

$$\beta_t = \sqrt{\frac{4m^* k_t}{1 + \left(\frac{\pi}{\ln e}\right)^2}}. \tag{9}$$

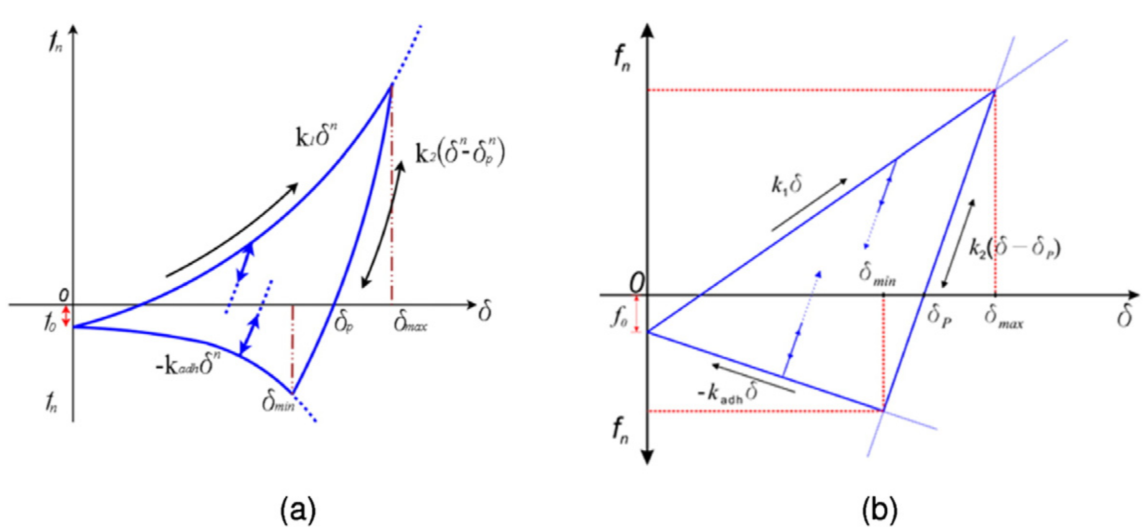

Fig. 1. Normal contact force–displacement function for the implemented model.