A hybrid DEM model suitable for micro and nano particulate systems incorporating long-range force contributions

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Abstract

Discrete element method (DEM) is a powerful tool for modelling the macroscopic and internal mechanics of particulate assemblies under mechanical loading. However, existing versions of DEM codes normally account for the inter-particle forces only when contiguous particles touch or overlap. In this paper, we examine the effects of long-range inter-particle forces acting between individual particles using DEM. Simulations were performed incorporating the contribution of repulsive force acting between particles even when the particles do not touch each other. When the particles touch/overlap with neighbouring particles, then inter-particle interactions are governed by a conventional linear spring-dashpot model; added to this is the contribution of normal force corresponding to zero separation distance between the particles. The simulations were of two types: (a), where no long-range forces were acting between particles (Type-0), and (b), where long-range forces were acting between particles (Type-1), which were entirely repulsive in nature. The long-range contact force data originates from hypothetical force curves similar to those obtained from Atomic Force Microscopy (AFM) experiments for powders with repulsive inter-particle interactions. Type-1 simulations are performed for three cases (A–C) of data describing force-separation curves that have identical approach and retraction loci. This preliminary study shows that the long-range force contribution significantly affects the macroscopic and internal behaviour of particulate assemblies under mechanical loading.

Keywords: Powder mechanics; Force-separation relations; Repulsive forces; Particulate materials; DEM

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1. Introduction

Granular materials are made up of large numbers of particles, which interact with one another at their points of contact. Forces are transmitted from one boundary to the other only through the inter-particle points of contact. Force transmission in particulate materials is vastly susceptible to the local arrangements of the particles, e.g. [1,2]. As a result, contact forces will usually be distributed in an intricate, uneven manner [3]. Recent computational studies on the micromechanical behaviour of granular assemblies show a closer link between the macroscopic shear strength characteristics and the manner in which force networks develop within granular assemblies, depending on the individual properties of grains and the packing conditions, e.g. [4,5,6,7]. Although a limited number of existing studies model the behaviour of cohesive powders, e.g. [4,6,8], the role of long-range forces on the micromechnical behaviour of powders is not yet fully understood. Among the existing models, JKR theory is commonly employed to model the normal interactions between cohesive powder particles, e.g. [6]. In JKR theory, the work done between surface attractions is equated to the work of deformation in elastic spheres. The resultant equation for adhesion between spherical particles involves a surface energy term, which is not always easy to measure experimentally. Further, powder-processing industries often deal with non-spherical particulate systems, and it is not yet clear how to model the behaviour of non-spherical powders, including the long-range interactions between the particles. When the particle sizes become small, particularly lower than the micron scale, then the role of long-range contribution is expected to play a dominant role in the behaviour of powder assemblies. Other simulation methods, such as molecular dynamics (MD), are valid only for (spherical) particle contacts,

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which are independent of one another [8]. Continuum models do not consider the discrete nature and anisotropic properties of contacting particulate materials. In this paper, we model the interaction between particulate systems using a hybrid DEM procedure, in which the long-range force-separation relation between particles can be directly specified as an input to the modelling. In real situations, for particles having sizes in the micro or nano regimes, the long-range force-separation relation can be measured using experimental techniques such as AFM.

2. Computer simulations

The simulations are carried out using the DEM, which was originally developed by Cundall and Strack [9]. The advantage of applying the DEM to granular materials is its ability to give more information about what happens inside the system. The method models the interaction between contiguous particles as a dynamic process and the time evolution of the particles is advanced using an explicit finite difference scheme. For the detailed information about the numerical methodology, the reader should refer to [9].

At the first instance, we considered mono-dispersed spherical assemblies consisting of about 8000 particles, and periodic conditions were specified along the boundaries. The initial assemblies were isotropic and homogeneous, with a dense packing condition (packing fraction = 0.574568). Three different cases of hypothetical long-range force-separation curves were considered, all repulsive in nature (cases A–C (Type-1), Fig. 1). For comparison purposes, we also performed a case study in which no long-range force was acting between particles (Type-0). The assemblies were subjected to uni-axial, quasi-static compression.

The total (normal) contact forces between two particles is the sum of the 'contact force' (corresponding to negative separation, i.e. positive overlap or touching) and the 'long-range force'. The force-displacement relation was as follows:

$$\mathbf{F}(\mathrm{k}) = -((\mathbf{F}\mathrm{n}+\mathbf{F}\mathrm{nfar}) * \xi(\mathrm{k}))+\mathbf{F}\mathrm{ttot}(\mathrm{k})+\mathbf{F}\mathrm{nd} \qquad (1)$$

The force between two particles, $\mathbf{F}(\mathrm{k})$ (k = 1, 2, 3 directional components), is the sum of normal forces (the contact force '**F**n' and the long-range force '**F**nfar', which both act in the normal 'ξ' direction), plus a tangent force '**F**ttot' due to tangential contact springs and tangential friction that act only when particles touch, plus a specified contact damping force '**F**nd'. That is, the long-range force is normal, and it is added to the contact force. When the particles are not touching, the contact force is zero, and the long-range force is interpolated from the input discretised data of Fig. 1. When two particles are touching (that is, when the separation is negative, and the overlap is positive), the long-range force is equal to the long-range force for zero separation. Also when two particles are touching, the contact force (both normal and tangential components) is computed with a simple linear spring-dashpot model: linear normal and tangential contact springs and a frictional slider. Slipping between particles would occur whenever the contact friction coefficient of 0.5 was attained. The ratio of tangential spring stiffness to normal spring stiffness is maintained as unity. Unit normal spring stiffness is assigned for determining contact forces normal to the

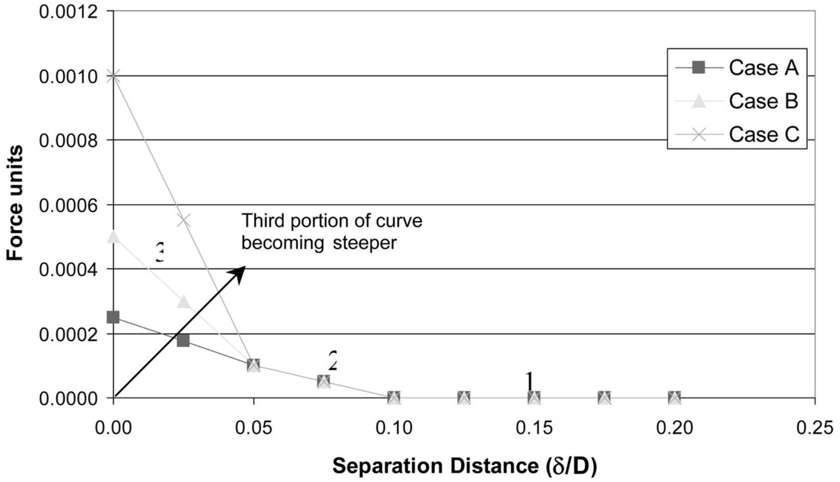

Fig. 1. Force-separation curves that were used for three cases (A–C) of Type-1 simulations. The separation distance δ is divided by the particle diameter D.

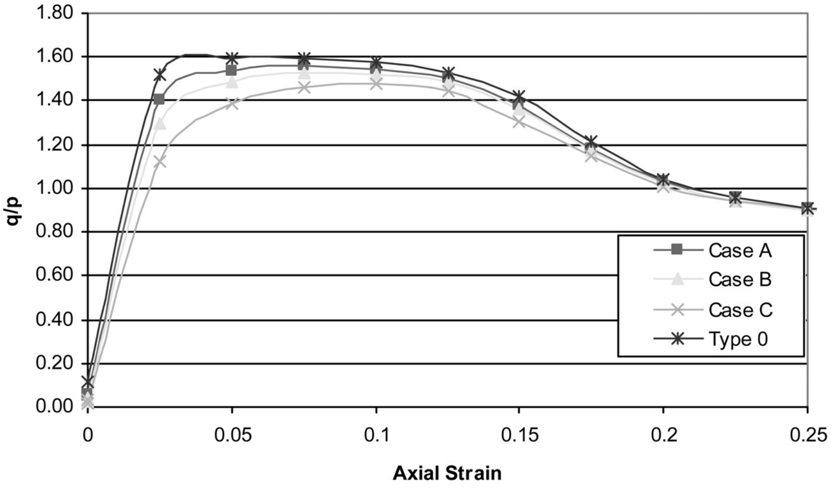

Fig. 2. Variation of deviator stress ratio q/p (q = deviator stress, p = mean stress) during compression.

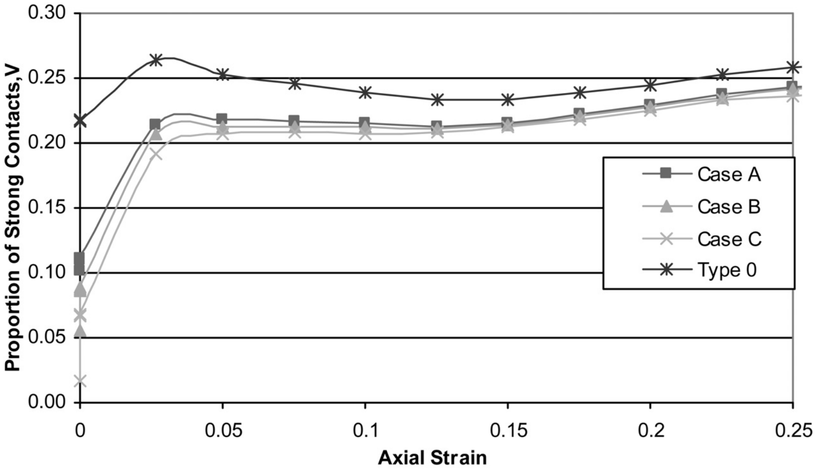

Fig. 3. Proportion of strong contacts during mechanical loading.

contact surfaces. This stiffness is multiplied by the indentation at the particle contacts to compute the contact normal force. As mentioned above, after the contact force is computed, it is added to the long-range force, to give the total force between the particles. In short, the simulation was set up to compute both long-range and contact forces, and it uses their sum to simulate particle movements and interactions.

3. Results and discussion

Here we present a selected number of microscopic and macroscopic features of the systems under study. The variation of macroscopic shear strength during compression, in terms of the deviator stress ratio q/p ($q = \sigma_{33} - \sigma_{11}$, $P = (\sigma_1 + \sigma_2 + \sigma_3)/3$), is presented in Fig. 2. From this chart it is evident that an increase in the gradient of the repulsion forces results in a decrease in the shear strength in particulate assemblies, particularly during pre-steady state. For the particulate system in which repulsive long-range forces are absent (Type-0), the shear strength is higher than that of a repulsive system (Type-1). Irrespective of whether a system is repulsive or not, all the systems attained a unique stress ratio q/p at the steady state.

Figure 3 shows the proportion of strong contacts, defined as the ratio of the number of contacts carrying

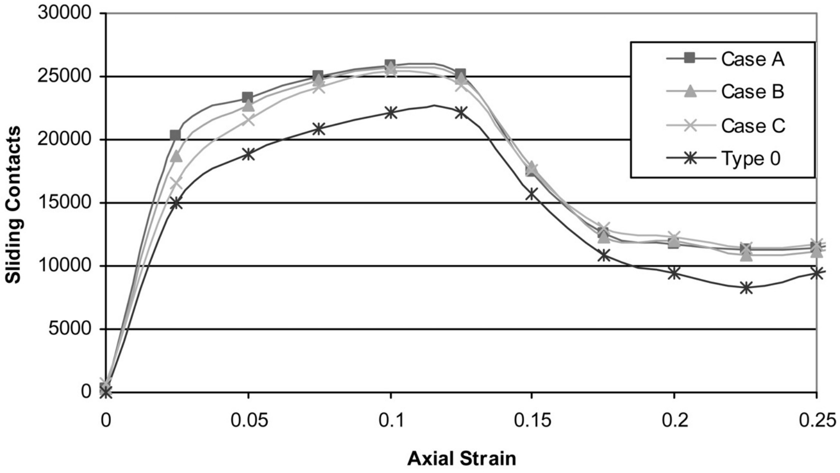

Fig. 4. Variation of sliding contacts during compression.

forces greater than the average normal force in the system to the total number of contacts at a particular stage of compression. Upon close investigation of Fig. 3, one can conclude that the proportion of strong contacts decreases as the gradient of particulate repulsive forces increases. Their ability to build up a strongly anisotropic network of strong contacts has a direct bearing on the macroscopic shear strength of particulate systems, and more details on this can be found elsewhere [4,6,7]. Figure 4 shows the number of contacts sliding in the assemblies during compression. As expected, the number of sliding contacts for system without long-range repulsion is lower than that of particulate systems having long-range repulsion. Further, for repulsive systems, an increase in the gradient of the repulsion resulted in a decrease in the number of contacts sliding during compression.

4. Conclusions

We presented a novel hybrid computational modelling of particulate systems, accounting the contribution of long-range force for studying the macroscopic and internal mechanics of repulsive particulate systems. Comparison of results for several features between repulsive and non-repulsive systems shows that the inter-particle long-range repulsive contribution plays a dominant role in the mechanics of particulate assemblies. These findings are significant and provide a platform for predicting more realisitc engineering behaviour of particulate assemblies at exceedingly small scales in future.

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