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On the force–displacement law of contacts between spheres pressed to high relative densities

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ABSTRACT

A finite element study of the interparticle force–displacement laws on contacts of spheres at conditions corresponding to compacts pressed to high relative densities is presented here. Under these conditions, the response of a contact can be affected by the presence of neighboring contacts. Finite element simulations of axisymmetric models of equispaced and equally loaded contacts show that the force–displacement law is not unique and depends on the number of neighboring contacts. The force at a given interparticle deformation is minimum for $Z = 2$ but at higher coordination numbers becomes larger after a critical deformation due to the interaction of the stress fields of neighboring contacts. This difference is magnified when the local porosity closes. Furthermore, numerical simulations of periodic arrays of spheres were conducted to assess the effect of loading path and the formation of new contacts on the response of existing contacts. In both cases, it was found that, the contact response depends on the overall triaxiality of the deformation of the particle. A new deformation fabric tensor is proposed based on the deformation and direction of all contacts on a particle. The first and second invariants of this tensor are used to characterize the triaxiality of the deformation on a particle. These results form the basis for more appropriate force–displacement laws at contacts that can be implemented in discrete element simulations for high density problems.

1. Introduction

Powder compaction can be modeled by continuum, micromechanical or discrete models. The most common constitutive model used in conjunction with finite element (FEM) analysis is the Drucker–Prager cap model (Coube and Riedel, 2000; Michrafy et al., 2002; Sinha et al., 2010; Sinka et al., 2003; Wu et al., 2005), which combines a Drucker–Prager failure line (Drucker and Prager, 1952) with a densification cap (DiMaggio and Sandler, 1971). Micromechanical models incorporate geometric parameters (i.e., coordination number, contact orientation) that have a significant effect on the mechanical behavior of the powder compact (e.g., Arzt, 1982; Fleck, 1995). Two classes of discrete models have been used: (a) Discrete Element Method (DEM) (Cundall and Strack, 1979; Heyliger and McMeeking, 2001; Martin et al., 2003; Redanz and Fleck, 2001; Thornton, 2000) that treats the compact as an assemblage of particles, which deform only at the contacts, and (b) multiparticle FEM (MPFEM), which is based on finite element discretization of particles (Gethin et al., 2003; Harthong et al., 2012; Procopio and Zavaliangos, 2005). Among these methods, DEM offers arguably the best combination of insight into particle level mechanisms and computational efficiency.

In this paper, we examine the force–displacement law governing the mechanical interaction of inter-particle contacts at large deformations. This law is the most important aspect of DEM models and is traditionally considered to be identical for all contacts in a pressed powder assembly. Contact models such as Hertz's (Hertz, 1882) and Storakers' (Storakers et al., 1997) are commonly assumed to describe the response of all contacts. The scope of this paper is to provide insight to the mechanical response of particles at high relative densities where significant interaction between neighboring contacts occurs, with the long term goal of extending the applicability of DEM models to that range.

2. Background

The normal force–displacement between elastic spherical particles, was derived analytically by Hertz (1882). This solution is based on the assumptions that: (a) a contact formed between two spheres is approximated by an elastic half-space loaded over

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a small circular area and (b) deformations are small. For plastically deformed contacts Storakers et al. (1997) developed an analytical model by extending the solution of Hill et al. (1992) for the indentation of a half-space by a rigid sphere. This is a *similarity solution* (Spence, 1968) in the sense that the solution is independent of the size of the indenter. In other words, velocities and strain rates are independent of the size of the contact area. Storakers' solution is based on the assumption of small deformations and uses a non-linear elastic material ($\sigma = k\varepsilon^{1/m}$, where k and m are a material constant and the hardening exponent respectively) in lieu of plasticity with the restriction of monotonic loading (e.g., Hutchinson, 1968; Rice and Rosengren, 1968).

Numerical simulations of a compressed row of spheres (Mesarovic and Fleck, 2000) showed that the Storakers' model is only valid during the earliest stages of contact deformation, and only for a large ratio of Young's modulus to yield strength ($E/\sigma_o > 1000$). Mesarovic and Fleck (2000) reported that the response of two spheres in contact comprises four distinct regimes: (1) elastic, small-strain, (2) elastoplastic deformation, (3) similarity (where the similarity solution is correct or close to the real response), and (4) finite deformation plasticity. They also stated that the transition between different regimes is affected by the ratio of the uniaxial yield stress σ_o to the modulus of elasticity E, and the ratio of the radii of the contacting particles.

Procopio and Zavaliangos (2005) performed 2D multiparticle finite elements simulations of compaction and showed that: (1) the force–displacement law at the contacts of discs is not unique but depends on the number of contacts formed in the particle and (2) there is an asymptote in the force–displacement curve that depends on the contact configuration in the particle and represents the fully dense limit at which the force tends to infinity for nearly incompressible particles. In other words there is interaction between neighboring contacts.

Skrinjar and Larrson (2007) performed 3D finite element simulations of the compaction of the body centered cubic array (BCC) and reported that the normal force deviates from the force developed at a contact formed between two spheres at moderate contact deformations. The deviation from the response of two particles in contact was attributed to the formation of additional contacts in the BCC configuration at the later stages of compaction.

Gonzalez and Cuitino (2012) developed an elastic model to address non-local phenomena by invoking the principle of superposition. They proposed that the displacement at a contact is the superposition of: (a) the direct effect of the force on that contact, and (b) the induced from neighboring contacts. The proposed idea is conceptually interesting as it challenges the uniqueness of the normal force–displacement law, but its consideration is restricted to small elastic contact deformations due to the use of the superposition principle.

To correct the typical deficiency of prior DEM models, which predict a finite stress at the fully dense limit, Harthong et al. (2009) developed a heuristic contact model that introduces the local relative density as an additional parameter in the force–displacement law. They proposed that the force developed on a contact should consist of two terms. The first term is associated with the force developed at a contact between two spheres, while the second is a singular term that takes into account the particle incompressibility, and is chosen to tend to infinity when the local porosity fully closes. This approach necessitates the calculation of local porosity using Voronoi tessellation.

Of interest to the current work is also the work of Frenning (2013), who proposed a force–displacement law describing a particle close to the full density limit. An analytical model was obtained by approximating the deformed spherical particle with a truncated sphere of size larger than the initial size of the particle (which is essentially an idea proposed by Arzt, 1982) and calculating the average contact pressure based on the volumetric deformation of the particle. The contact force is assumed to be a function of a constant parameter H and the contact area. Therefore, for a given contact area the force is unique. In that work it was also discussed that the force displacement response is initially affected by the merging of plastic zones under contacts and finally by the closing of the pores.

The current study focuses on the inter-particle contact response up to high relative densities, where the response of a particular contact is affected by the existence of neighbor contacts. Finite element simulations were conducted in order to elucidate the physical mechanisms that control the contact response under an overall isostatic pressing. Furthermore, numerical simulations of regular arrays were conducted to assess the effect of non-isostatic loading path and the effect of formation of new contacts on the response of existing contacts.

3. Constitutive model, FEM implementation and dimensionless analysis of the contact problem

3.1. Axisymmetric finite element mesh

The geometry of a conical sector deforming against a frictionless rigid wall represents the unit cell of a contact, see Fig. 1(a). Points on the side of the conical sector are constrained to move only along this surface. The presence of neighboring contacts is enforced in a way that represents equispaced and equally loaded contacts on a spherical particle. Fig. 1(b) shows the definition of the basis terminology that will be employed throughout the text (interparticle deformation, contact radius, etc.).

The surface area, S in the undeformed state is a function of the coordination number, Z:

$$S = \frac{4\pi R^2}{Z} \qquad (1)$$

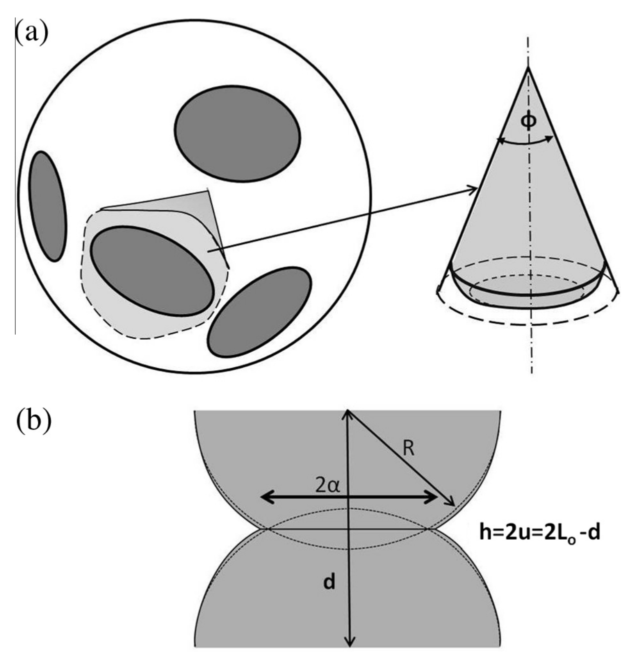

Fig. 1. (a) Geometric approximation of a contact on a spherical particle with coordination number Z for which contacts are equispaced and identically loaded (b) schematic and basic variables (α = contact radius, d = center-to-center distance of deformed particles, h = particle "overlap", and u = interparticle deformation) between two spherical particles in contact of radius R. The reference center-to-center distance L_0 is taken at the point that the contact just begins to form.