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An experimental evaluation of discrete element simulations of confined powder compression using an extended truncated-sphere model

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ABSTRACT

Confined compression of powders consisting of millimetre-sized granules was studied numerically with the discrete element method (DEM) and experimentally using a materials tester. A novel contact model was used, referred to as the extended truncated-sphere model, which is based on a geometrical analysis of the particle shape coupled with a contact pressure that varies with volumetric particle strain. The model accounts for plastic particle densification and utilises Voronoi cells to estimate the void space surrounding each particle. Simulations were performed both with and without an account of plastic particle densification, using experimentally estimated values of hardness and literature values of bulk moduli as input. An adequate agreement between simulations and experiments was obtained for beds of ductile particles, but the correspondence was less satisfactory for ductile-brittle ones. The results indicate that a residual porosity remained in the particles also at the highest applied pressures in both cases. It was concluded that the novel extended truncated-sphere model is suitable for and provides insight into the problem of simulating confined powder compression at large strains. However, reliable results will likely not be obtained for fragmenting particles unless a way be found to describe particle fracture.

1. Introduction

A considerable amount of research done in the pharmaceutical area has during many years focused on reducing the variability of products such as tablets manufactured by confined compression. It is therefore of utmost importance to gain an understanding of the underlying causes for the variation. Significant progress has been made by numerical methods but an improved understanding of the compression process including essential parameters for accurate descriptions of the various stages during compression is still needed. A promising and important tool often used for simulations in the pharmaceutical sciences is the discrete element method (DEM) [1]. The DEM enables simulations at the particulate level and uses a soft-particle approach where the contacts are modelled by a particle overlap.

The most commonly used contact models in DEM simulations of confined compression of granular materials are of an elastoplastic or a purely plastic type. Well-known examples include the model proposed by Storåkers et al. [2] that emanates from a similarity analysis of inelastic contacts, the model put forward by Thornton and Ning [3] that is based on a truncation of the Hertzian pressure distribution at a certain yield pressure, and the model of Vu-Quoc and Zhang [4] that utilises an additive decomposition of the contact radius into elastic and plastic parts. A more recent example is the model developed by Brake [5]. These models generally predict a largely linear increase in the contact force with increasing strain, except at very small strains, where the elastic Hertzian response makes the force–displacement relation nonlinear. In addition, simplified hysteretic spring models are sometimes also used, as originally proposed by Walton and Braun [6] and elaborated upon by Luding el al. [7]. Such models also predict a linear increase in force during loading.

However, the inherent assumption of contact independence made in the DEM and the aforementioned contact models is not justified at the large strains occurring during the late stage of compression (exceeding relative densities of about 0.8) [8,9], rendering simulations of the elastic compact deformation problematic. This issue has been addressed in several ways. The analytical model presented by Harthong et al., based on curve-fitting to a meshed discrete element (MDEM) compression simulation, satisfactorily described the large strain incompressibility in DEM simulations [10]. In the model, the change in local relative density during compression was calculated from the corresponding volume change of Voronoi cells. This model has further been elaborated upon by Jerier et al. [11] and Harthong et al. [12]. A related, nonlocal contact model was developed by Gonzalez and Cuitino [13] who utilised the superposition principle to infer contact interactions for purely elastic particles. To model the large strain incompressibility in an average sense, keeping the notion of independent contacts, a maximal plastic overlap was introduced in the truncated Hertzian contact model [3,14]. The maximal plastic overlap defines the particle overlap at which elastic deformation is initiated [14]. A similar force–displacement relation was used by Olsson and Larsson [15] (cf. their Fig. 9b) who interpreted the increased stiffness as resulting from hardening occurring

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at a certain magnitude of the plastic strain. An analytical model proposed by Frenning [16] accounts for contact dependence and highlights the bulk modulus and the particle hardness as important parameters for describing the contact pressure evolution at low and intermediate strains. As originally suggested by Arzt [17], the deformed particle shape was described as a truncated sphere. The potential of this truncated-sphere contact model was established by an adequate correspondence to finite element simulations. The bulk modulus is preferable over the Young's modulus for defining the particle volume changes as the bulk modulus provides a measure of the resistance to hydrostatic particle compression. The plastic hardness is suitable for describing the local plastic deformation at particle contact. However, the truncated-sphere model accounts only for the initial particle compression, i.e. before contact impingement occurs; thus limiting the plastic deformation propensity. To account for the plastic incompressibility evident at large strains an extension of the model with Voronoi cells is appropriate.

The aim of this work was to extend the truncated-sphere model [16] so that it can be used in DEM simulations of confined compression and to compare its predictions of bulk compression to experiments. Granulated powders comprising millimetre-sized granules of a ductile (formed from microcrystalline cellulose) or a ductile-brittle (formed from a mixture of microcrystalline cellulose and lactose) character were used as model systems.

2. Theory

In our previous work [16], a simplified model of the response of elastoplastic particles subjected to multiple simultaneous contacts was proposed. The model rested on two key assumptions, namely that the deformed particle shape could be approximated as a truncated sphere and that the contact areas could be translated to contact forces via an effective hardness $\overline{H}$. Although these assumptions resulted in a model that adequately captured numerical data for small to moderate (volumetric) strains, extensions are needed for large strains for two primary reasons. Firstly, the contact areas cease to be circular because of contact impingement and, secondly, the average contact pressure will increase beyond the hardness as a result of particle confinement. Here, such an extension is presented that utilises Voronoi polyhedra to estimate the particle volume and contact areas at large strains. In addition, a modification of the model that allows for plastic volume reduction of porous particles is proposed. For simplicity, we will assume that a mean contact pressure $\overline{P}$ can be used to relate the contact area to the normal force throughout the deformation, and hence write

$$F_i = \overline{P} S_i \tag{1}$$

where F_i and S_i are the normal force on and surface area of contact i, respectively. Eq. (1) represents an effective description that remains valid even though the contact pressure need not be uniform throughout the deformation.

Contact pressure: As illustrated in Fig. 1a, we consider the average contact pressure $\overline{P}$ to be a function of the volume V of the Voronoi polyhedron and identify three regions separated by two limiting volumes V_1 and V_2. For small volumetric strains, i.e., large values of V ($V > V_1$), the average contact pressure $\overline{P}$ was put equal to $\overline{H}$ as in the model in its original form. For large volumetric strains ($V < V_2$), the determination of $\overline{P}$ was based on the definition of the bulk modulus κ of the dense material constituting the granules, using the Voronoi volume V as an estimate of the current particle volume. An interpolation was used for intermediate volumetric strains ($V_2 < V < V_1$). Specifically, $\overline{P}$ was expressed as follows:

$$\overline{P} = \begin{cases} \overline{H} & \text{if} \quad V > V_1 \\ \overline{H} + K(V_1 - V)^{\alpha} & \text{if} \quad V_2 < V < V_1 \\ \kappa\left(1 - \dfrac{V}{V_s}\right) & \text{if} \quad V < V_2 \end{cases} . \tag{2}$$

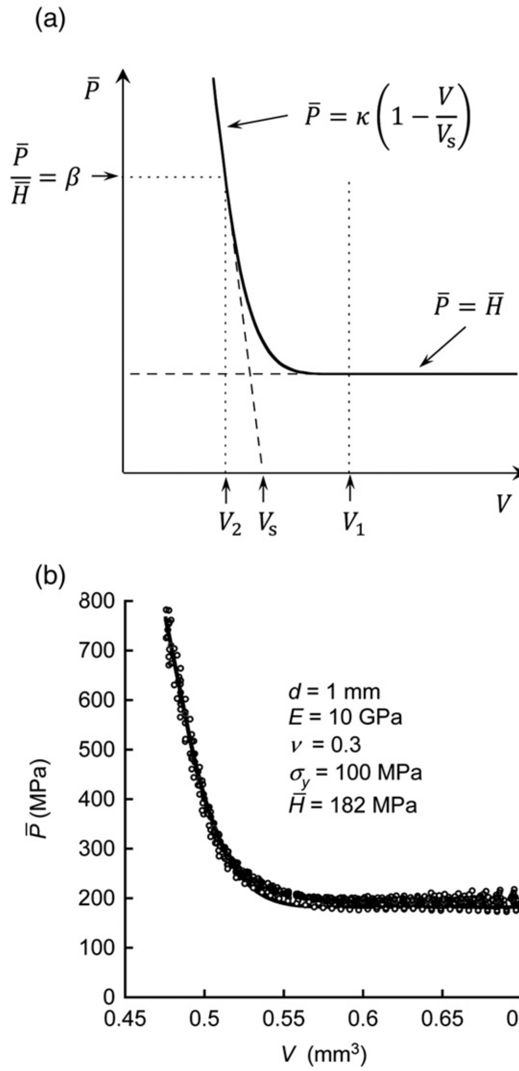

Fig. 1. Dependence of the mean contact pressure $\overline{P}$ on the Voronoi volume V. (a) Schematic illustration indicating the influence of the effective hardness $\overline{H}$ and bulk modulus κ using the parameters β, V_s, V_1 and V_2 described in the text. (b) Comparison between $\overline{P}$ as obtained from Eq. (2) using the parameter values $\alpha = 5$ and $\beta = 3$ (thick solid line) and numerical results (symbols) from triaxial loadings with different loading rates in the three spatial directions [16]. Parameter values are indicated in the figure (d = particle size, E = Young's modulus, ν = Poisson's ratio, σ_y = yield stress and $\overline{H}$ = effective hardness).

Here, K and α are constants and $V_s = (1 - \phi_0)V_{p0}$ is the volume of the solid material that constitute the particle (ϕ_0 and V_{p0} are the initial particle porosity and volume, respectively). As already indicated, V_1 and V_2 denote the upper and lower limits of the region where the contact pressure is interpolated, respectively.

Assuming that the interpolation ends at a pressure-to-hardness-ratio β (i.e., $\overline{P}/\overline{H} = \beta$ at $V = V_2$; see Fig. 1a), the limiting volume V_2 can be expressed as

$$V_2 = \left(1 - \frac{\beta \overline{H}}{\kappa}\right) V_s. \tag{3}$$

If one considers the exponent α as a known parameter, the limiting volume V_1 and the constant K can be determined from the condition that P and the derivative $\mathrm{d}P/\mathrm{d}V$ both be continuous at V_2, implying that

$$V_1 = \left(1 - \frac{\overline{H}}{\kappa}\right) \alpha V_s - (\alpha - 1) V_2 \tag{4}$$