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Mechanical behaviour of ideal elastic-plastic particles subjected to different triaxial loading conditions

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The contact force development for two types of polymeric elastoplastic particles subjected to different triaxial loading conditions was studied experimentally utilising a unique triaxial testing apparatus. In order to evaluate the experimental results, a finite element analysis was performed. The experimental findings highlighted the importance of contact dependence, which manifested itself in two principally different ways. Firstly, a reduced stiffness was observed when plastic deformation ceased to be fully contained, which, depending on the loading conditions, occurred at an engineering strain of about 5–10%. Secondly, a markedly increased stiffness was observed when particle confinement inhibited further plastic deformation, making elastic volume reduction the predominant deformation mode. The experimental results could be well reproduced by the numerical simulations, provided that isotropic hardening was included in the elastoplastic model. In an attempt to invariantly describe the data, a nominal contact pressure was determined as a function of the volumetric constraint of the particle. This resulted in an adequate collapse of results obtained for different loading conditions onto a single master curve at large volumetric constraint. In summary, this paper should be considered as a step along the pathway towards our long term goal of introducing novel and improved contact models.

1. Introduction

Confined powder bed compression is a common procedure for shaping products in several industries, e.g. in metallurgy, ceramics and pharmaceutics. In order to adequately predict the performance of the compaction process and hence the quality of the end product, there is an obvious need for accurate models. Traditionally, models inferred from the bulk behaviour of the powder bed, such as the ones introduced by Heckel [1] and by Kawakita [2], have been employed. However, such models reveal very little of the behaviour of individual particles during compaction. Therefore, bottom-up models involving material data from indentation experiments have been derived. Here we find, for example, the model proposed by Hill et al. [3] as well as the similarity analysis proposed by Storåkers et al. [4]. However, the increased complexity when evaluating confined powder compression from a bottom-up perspective has been highlighted by e.g. Fischmeister and Arzt [5], who pointed out the imminent phenomenon of interacting contacts, which they referred to as *geometrical hardening*. Accordingly, when evaluating the similarity analysis performed by Storåkers et al., Mesarovic and Fleck found that contact interaction comes into play rather early during compaction, rendering contact models derived from analyses of isolated contacts invalid when approaching relative densities corresponding to a degree of compression where the formation of an integral compact takes place [6].

Several methods have been applied to model particle deformation after the onset of contact–contact interactions. Utilising the linearity of elastically deforming bodies, Gonzalez and Cuitiño invoked the superposition principle to describe simultaneously emerging contacts on elastic spheres [7]. Harthong et al. introduced an incremental formulation with a stiffness that contained a singular term that depended on the local relative density. Voronoï tessellations were used in order to determine the local geometry (i.e., the relative density), and hence the degree of contact dependence at each instance [8]. Montes et al. approached the geometrical limitations through applying a model involving the effective pressure [9]. Frenning extended this idea by introducing a model where the displacement of material caused by the particle overlap is compensated for by increasing the original particle radius as the compression proceeds [10,11]. Of notable relevance is also the endeavour of Tsigginos et al. to devise a fabric tensor with the intention of finding a way to describe each contact independently of the loading conditions [12].

Currently, in developing novel contact models, numerical methods such as the finite element method (FEM), as well as the meshed discrete element method (MDEM) are often utilised [8,10,12–15]. As an alternative, we have experimentally addressed confined compression of single particles, involving several different materials [16,17]. Thus far, we have only employed hydrostatic conditions. However, in a powder

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bed subjected to uniaxial compression, as during tableting, the loadings exerted on an individual particle will be non-hydrostatic in most cases. Empirical proof for this has been provided for example by Alderborn et al. [18,19] who during tableting observed higher aspect ratios ("flakiness") of the individual granules with increasing compression pressure. This phenomenon is expected to be of importance for the evolution of the force at each contact. Simulations have shown, for instance, that contact stiffness on less deformed contacts is significantly higher than at the more deformed ones when compressing non-hydrostatically [10,12]. Our aim here is therefore to experimentally characterise the contact force development of single particles when subjected to a range of different triaxial loadings in order to gain insights into the mechanics of the particle under confined conditions. From the obtained results, we set out to find a way of representing the evolution of the contact pressure invariantly, regarding both triaxial loading condition and whether the contact is dominant or secondary. In order to evaluate the experimental results, a finite element analysis is also performed.

2. Materials and methods

2.1. Materials

Spherical cellulose acetate (CA) and polytetrafluoroethylene (PTFE) particles (nominal diameters: 2.00 mm and 1/16 in. $\approx$1.59 mm, respectively) were obtained from *Engineering Laboratories Inc.* (Oakland, NJ, USA).

2.2. The triaxial testing apparatus

The experiments were performed using a slightly modified version of the triaxial testing apparatus described in Ref. [16]. Briefly, the apparatus contains three pairs of punches where the punches in each punch pair are oppositely oriented. Further, each pair of punches is oriented perpendicularly to the other two pairs. For each pair of punches, one punch is axially mobile while the opposing punch is stationary. The punches are allowed to slide past one another, so that the side lengths of the cuboidal cavity between the punch surfaces can be changed independently of each other, enabling a particle placed in this space to be subjected to different triaxial loading conditions. For this to be possible, precise coordination of the punch motions is necessary, since the axial motion of one punch requires lateral motions of two adjacent and perpendicularly oriented punches. The axial movement of the three punches was performed using linear actuators (*M238.5PL, Physik Instrumente GmbH & Co, Karlsruhe/Palmbach Germany*). Detailed descriptions of the apparatus design, working principles and working action are given in Appendix A and in Ref. [16].

The punch positions were detected by position sensors integrated in the linear actuators and the forces exerted on all six punches were recorded by six 500 N force transducers (*ELAF-T1-M-500N-AC, Measurement Specialties, Les Clayes-sous-Bois, France*). The signals from the position sensors and force transducers were registered by in-house computer software designed in LabVIEW 2013 (*National Instruments, Austin, TX, USA*). The recorded punch positions were corrected for deformations in punches and other parts of the apparatus. The force–deformation characteristics used for this correction (linear and in the order of 300 μm/N) were determined in a separate procedure, as described in Ref. [16].

2.3. Experimental procedures

For both particle types, a total of nine loading cases were investigated (identical to those investigated numerically by Frenning [10]; see Table 1). For each loading case and particle type, 5 independent measurements were performed. In each of the loading cases except the hydrostatic one, two of the axes were set to compress at the same rate, whereas the third was set to compress either faster or slower than the other two. The slowest punch was programmed to move at a rate of 1.2 mm/min and the loading rates of the other punches were adjusted with this as a reference. Throughout the paper, when speaking generally of loading conditions with two fast and one slow punch, we will use the denotation *A:A:B*, whereas *A:B:B* will be used when referring to the cases with one fast and two slower punches. The hydrostatic case will serve as a reference for all the other cases and hence falls into both categories.

Table 1
The investigated loading cases and the corresponding loading rates along the respective axis.

Loading condition	*Loading rate x (mm/min)*	*Loading rate y (mm/min)*	*Loading rate z (mm/min)*
5:5:5 (hydrostatic)	1.2	1.2	1.2
5:5:4	1.5	1.5	1.2
5:5:3	2.0	2.0	1.2
5:5:2	3.0	3.0	1.2
5:5:1	6.0	6.0	1.2
5:4:4	1.5	1.2	1.2
5:3:3	2.0	1.2	1.2
5:2:2	3.0	1.2	1.2
5:1:1	6.0	1.2	1.2

2.4. Numerical model

Simulations were performed using a finite-strain hyperelastoplastic model implemented in the commercial finite-element software COMSOL (*version 5.2a; COMSOL AB, Sweden*). In brief, the elastic response was derived from a neo-Hookean strain energy that depended on the Lamé constants λ and μ (these constants were calculated from the small-strain Young's modulus E and Poisson's ratio ν in the standard manner). The onset of plastic deformation was governed by a von Mises yield function with isotropic hardening of the Ludwik type [20]. Hence, yielding occurred when the effective stress (also known as the von Mises stress) reached the yield stress σ_y defined as

$$\sigma_y = \sigma_{y0} + k\varepsilon_{pe}^n = \sigma_{y0}\left(1 + \alpha\varepsilon_{pe}^n\right) \tag{1}$$

Here, the initial yield stress σ_{y0}, the strength coefficient k and the hardening exponent n are constants. The effective plastic strain $\varepsilon_{\rm pe}$ is calculated from the logarithmic plastic strain in a similar manner as the effective stress is calculated from the deviatoric Cauchy stress. The non-dimensional ratio $\alpha = k/\sigma_{y0}$ has been introduced in the last member. The chosen values for the aforementioned parameters can be found in Table 2.

Triaxial compression of initially spherical single particles (initial radius R) was modelled and contact between the particle surfaces and the punches was enforced by using the penalty method, ensuring that the penalty factor was large enough that negligible penetration occurred. Taking symmetry into account, one octant of the particle was discretised into about 16 000 first-order tetrahedral elements. Negligible friction between the particle and the punches was assumed.

Table 2
Parameters used in the numerical simulations.

	R (mm)	E (GPa)	ν (−)	σ_{y0}(MPa)	α (−)	n (−)
CA	1.00	4.0	0.4	37	2.4	1.25
PTFE	0.79[a]	0.5	0.46	15	2.4	1.25

R = Initial particle radius; E = Young's modulus; ν = Poisson's ratio; σ_{y0} = initial yield stress; α = strength coefficient to initial yield stress ratio; n = hardening exponent

[a] Nominally 1/32 in.