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Three-dimensional discrete element models for the granular statics and dynamics of powders in cavity filling

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ABSTRACT

Rapid granular flow from a moving container and angle of repose formation were investigated by numerical simulations using the discrete element method (DEM) and experiments. Grain models of various geometrical complexity were studied and their ability to reproduce the experiments in those regimes was explored. The predictive power of the most realistic model for gravity driven cavity filling was assessed. Good agreement between computed and measured density distributions within the filled cavities provides a basis for numerical process variations aiming at homogenized density distributions. The effect of numerical coarse graining was found to be negligible for all properties of interest provided that force laws are scaled properly and corrections for boundary effects are taken into account. The proposed scaling was tested for a certain set of force laws but could be applied to different DEM forces as well. An analytic mass flow law for powder discharge from a moving container was derived and verified by our DEM simulations.

1. Introduction

Powder technological die compaction and sintering (German, 1996) are important techniques for the mass production of geometrically complex parts. The standard processing route consists of three steps (Wu and Cocks, 2004; Schatt and Wieters, 1997). It starts with the filling of the die (a cavity with the negative shape of the part): the powder is poured from a reservoir hopper through a hose into a moveable container (feeding shoe) and then the shoe passes the die one or more times thereby delivering powder into it. This first step is followed by uniaxial compaction with punches resulting in a so-called green body with a very brittle consistency. The green body is ejected from the cavity and placed in a furnace for the final sintering step: thermal activation below the melting point leads to the formation and growth of necks between adjacent grains and eventually to a fully dense structure (German, 1996).

Generally, the filling of the die and the subsequent compaction lead to inhomogeneous distributions of the powder in the green body. Although the contribution of die compaction to inhomogeneities is often considered to be the more important one, die filling can also make substantial contributions, which, depending on the die geometry, are not levelled out during compaction (Coube et al., 2005). For example, shallow part geometries such as flat discs are usually filled rather inhomogeneously, while the compaction step is unproblematic.

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Inhomogeneous green densities lead to inhomogeneous shrinkage during sintering and therefore to distortions of the sintered part. Another frequent problem in powder technology is cracking, which most often occurs at different stages of the compaction and ejection process (Coube and Riedel, 2000). Reliable simulation tools for the whole process chain would help to cope with these everyday problems in powder technology. Especially the simulation tool for die filling presented here is beneficial in two ways. On the one hand it allows minimizing inhomogeneities in fill density by optimized process parameters such as shoe kinematics. On the other hand, if inhomogeneities are not avoidable, it is advantageous to know them in advance, so that the resulting sinter distortions can be compensated in the tool geometry or at least minimized by a suitable press kinematics.

Unfortunately, simulations of die filling in the literature are restricted to using the finite element method (FEM) (Riera et al., 2005) or to two-dimensional (2D) discrete element method (DEM) powder models (Wu et al., 2003a; Wu and Cocks, 2006). Both methods provide at most a generic understanding of the filling process. Quantitative predictions require enhanced realism in the modelling of the granular motion. The present article provides a contribution into this direction by exploring the performance of three-dimensional (3D) DEM models in a set of representative die filling scenarios.

Seminal works on discrete element modelling of powders and grains were carried out by Cundall and Strack (1979), Campbell and Brennen (1985), Walton and Braun (1986), Haff and Werner (1986), and Gallas et al. (1992). A range of investigations exists focusing on hopper outflow (e.g. Langston et al., 1994, 1995, 1996; Ristow, 1997; Hirshfeld et al., 1997; Cleary and Sawley, 2002) and angle of repose formation (e.g. Lee and Herrmann, 1993; Pöschel and Buchholtz, 1993; Buchholtz and Pöschel, 1994; Zhou et al., 2001). However, no studies aiming at a comprehensive 3D powder modelling, i.e. describing more than a single regime with one model parameterization, are known to the authors. To our knowledge the present study is the first one using 3D DEM models for the simulation of die filling. Our main goal was the description of granular flow and settlement in realistic cavities without the constraints in particle rearrangement arising from corresponding 2D models.

The behavior of a DEM powder model crucially depends on the applied force laws, the grain shapes and the grain size distribution function. For overviews of DEM force schemes see e.g. Schäfer et al. (1996), Luding (2006), Kruggel-Emden et al. (2007), and Zhu et al. (2007). An intrinsic difficulty of die filling simulations with 3D grain models is the large number of particles involved. Limitations in current computing power and memory impede a description of macroscopic filling scenarios using the experimental grain sizes. The use of larger grains represent the only route to circumvent these difficulties. In the present article, coarse grained spherical and non-spherical powder models are used. Basically such a coarse grained powder constitutes an effective medium that should exhibit the same dynamic and static properties as the experimental granular material. The feasibility and the limitations of the coarse graining are elucidated and fundamental scaling rules for the intergranular forces are derived.

Free parameters in the force expressions are adjusted by matching to meaningful experiments. Compared to numerous investigations on compaction and sintering only few experimental studies on die filling have been carried out. Bocchini (1987) found that the integral filling densities decreases for small die sizes. Rice and Tengzelius (1986) tested different devices for their ability to classify powder flowability and integral filling density. Hjortsberg and Bergquist (2002) observed density variations in a narrow ring cavity. Wu et al. (2003b) studied influences of cavity geometry and shoe kinematics on the integral filling density. In subsequent studies the same authors (Wu and Cocks, 2004; Sinka et al., 2004; Schneider et al., 2005) developed the concept of a critical shoe velocity for complete filling. Burch et al. (2007) observed spatial density inhomogeneities depending on cavity geometry and shoe kinematics using X-ray computer tomography. Wu et al. (2003a) were the first to compare experiments with 2D DEM simulations and to investigate the influence of escaping air and cavity geometry on the die filling process.

Since these studies differed in their setups as well as in the considered powders, we decided to conduct our own experiments in order to establish a coherent database for the force fitting. The focus was laid on dynamic (outflow rates from a moving container) as well as static (angle of repose) properties of the powder. The parameters in the force laws were optimized to reproduce either the dynamic or static powder properties. The quality of the resulting parameter sets was assessed by cross-validation, i.e. to predict the angle of repose with forces parameterized with the experimental outflow rates and vice versa. A reliable description of both (i.e. dynamic and static) regimes is important for an accurate calculation of final density distributions in die filling, since outflow rates determine the amount of powder that enters the cavity and the angle of repose is related to the settlement of the powder in the cavity.

This article is organized as follows. The experiments for adjustment and validation of the powder models are described in Section 2. The force models are explained in Section 3. The description of the experimental results is given in Section 4 followed by a section about the parameter adjustment (Section 5) and a systematic study of coarse graining effects (Section 6). In Section 7 the optimum powder model is employed to predict density distributions of realistic die filling scenarios. The comparison with corresponding experiments allows for a critical assessment of the predictive power of our DEM model. The article ends with a general conclusion in Section 9 and Appendix A reports on the derivation of an analytic expression for the mass flow from a moving container—an extension of the Beverloo equation for hopper outflow (Beverloo et al., 1961; Nedderman et al., 1982).

2. Experimental setup

A model system as shown in Fig. 1a was setup. Its design resembles a similar device presented in Wu et al. (2003b) and Wu and Cocks (2004). A perspex filling shoe (32 mm long, 50 mm wide, 37 mm high) moves over an exchangeable polished