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Modeling yield properties of compacted powder using a multi-particle finite element model with cohesive contacts

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ABSTRACT

The multi- particle finite element method (MPFEM) was used to simulate the yield properties of compacted powders with cohesive contacts. A suitable representative volume element (RVE) of monodisperse, spherical, deformable particles was created to be implemented into a commercially available finite element code. New efficient periodic boundary conditions were proposed to compute representative properties of the volume at limited computational costs. A contact model was introduced, which includes repulsive forces, friction forces and cohesion forces. As a result, the proposed model is capable of considering tensile strength in a MPFEM setting, which was not attainable in related published work.

We present extensive parameter studies to demonstrate the performance of the proposed RVE and to find the optimal balance between accuracy and computational speed. The minimum mesh fineness and the minimum number of particles in the RVE were determined during convergence studies. The employed explicit integration scheme was enhanced by means of mass scaling. The optimized model was used to predict the strength of compacted powders. A simple analytical expression was fitted to the numerical predictions to describe the uniaxial tensile strength and the uniaxial compression strength as a function of the powders' relative density and the cohesion strength of the contacts. A general form of a yield surface was proposed to describe the yield properties for generic load cases, which can be applied to different relative densities and cohesion strengths. As a result, we showed that the yield surfaces grow with increasing relative density, while they change their shape with increasing cohesion strength. The obtained yield surface results in the Drucker-Prager/Cap model in case of low cohesion, whereas it has an elliptical shape in case of high cohesion. The proposed analytical form of the yield surface is capable of describing both cases.

1. Introduction

Cold compaction of powder is important for many industrial processes, e.g., for the production of green bodies before sintering of metals, ceramic parts in mechanical engineering, pellets for mineral or animal food industry or the production of tablets in the pharmaceutical industry [1–4]. The goal of powder compaction is to reduce the volume of the powder, increase the flowability or to create a part of a certain shape and size.

The final powder compact requires a minimum strength as otherwise it would disintegrate during processing, transportation or storage. The strength of a compact depends on both, material and process parameters. Important material parameters are the chemical composition of the primary particles (and their mechanical properties), as well as the particles' size and shape. Furthermore, the material properties are influenced by the environmental conditions, e.g., temperature and humidity. The process parameters include the geometry of toolings and dies, the compaction stress or strain, as well as on the compaction force-versus-time profile, which depends on the control strategy of the compaction machine. Experiments can be used to adjust the process to get the desired compact properties. Commonly, this is time-consuming, as process parameters change often, e.g., the geometry of the machine tools or the powder properties. Hence, reliable numerical models to predict the properties of compacts with simulations are crucial.

Phenomenological models for powder compression have been in use for many decades. The Heckel equation [5] and the Kawakita [6] equation are, among many other approaches, most commonly used nowadays. Recent studies dealing with these equations were reported [7–

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9]. Both equations correlate the applied pressure with the relative density (or porosity) of the powder compact. Another noteworthy phenomenological model is the Ryshkewitch-Duckworth [10] equation which correlates the relative density of a powder compact with its strength, which is of higher interest in practical situations. Recent studies using this equation are reported in [11, 12]. All models have in common that the introduced constants are empirically adjusted by means of compaction experiments and force measurements. The disadvantages of these phenomenological approaches are the minimal mechanistic understanding of the process and the lack of information about the strength of the final compact. Moreover, the parameters determined for one material (or one size fraction) are not valid for other materials.

There also exist some analytical models in the literature which describe the compaction process. We mention here exemplarily [13, 14] with analytically derived flow surfaces and [15] with the authors considering the densification during compaction and sintering theoretically. Although very interesting in principle, the disadvantage of analytical models is their oversimplification. Most often, affine motion has to be assumed and the description of particle deformation is very difficult. Such assumptions limit the practical applicability of these models.

In recent years, two numerical methods became important for powder flow simulations, which are the discrete element method (DEM) and the finite element method (FEM). In DEM every single particle is modeled and numerically tracked. The interaction forces between particles are computed based on the overlap of the particles (soft-sphere model) and Newton's equations of motion are solved for the particles' acceleration, velocity and position. As a result, the rearrangement of particles during compaction can be efficiently modeled. Recent investigations in this area were carried out, e.g., by [16–20]. Note that particle deformation, which is dominant at higher densities of the powder compact, are commonly not taken into account. Furthermore, the fully discretized nature of DEM entails high computational costs and practically limits the number of particles to fewer than 10 million. In contrast, in classical FEM simulations powders are described as a continuum, i.e., the discrete nature of the particles is not implemented. This renders the method to be much more efficient than DEM. Recent studies include [21–23]. However, in FEM a material model is required to connect the stress and the strain of the material. The determination of such material models, including the yield surface, is a difficult and cumbersome task.

Several models for yield surfaces connected to powder compaction can be found in the literature. The Drucker-Prager/Cap model based on [24] is one of the most often used yield surfaces. It is conceived for pressure-dependent materials and widely used for geological materials, powders, polymers, concrete, foams and other substances. Another common model is the so-called modified Cam-Clay model [25], which was developed for soft soils. Its yield surface is an elliptical curve. Both models are compared in the recent work of [26]. The shape and the evolution of the yield surfaces are shown in the p-q diagrams (equivalent pressure stress p and von Mises equivalent stress q) (see Fig. 1). With

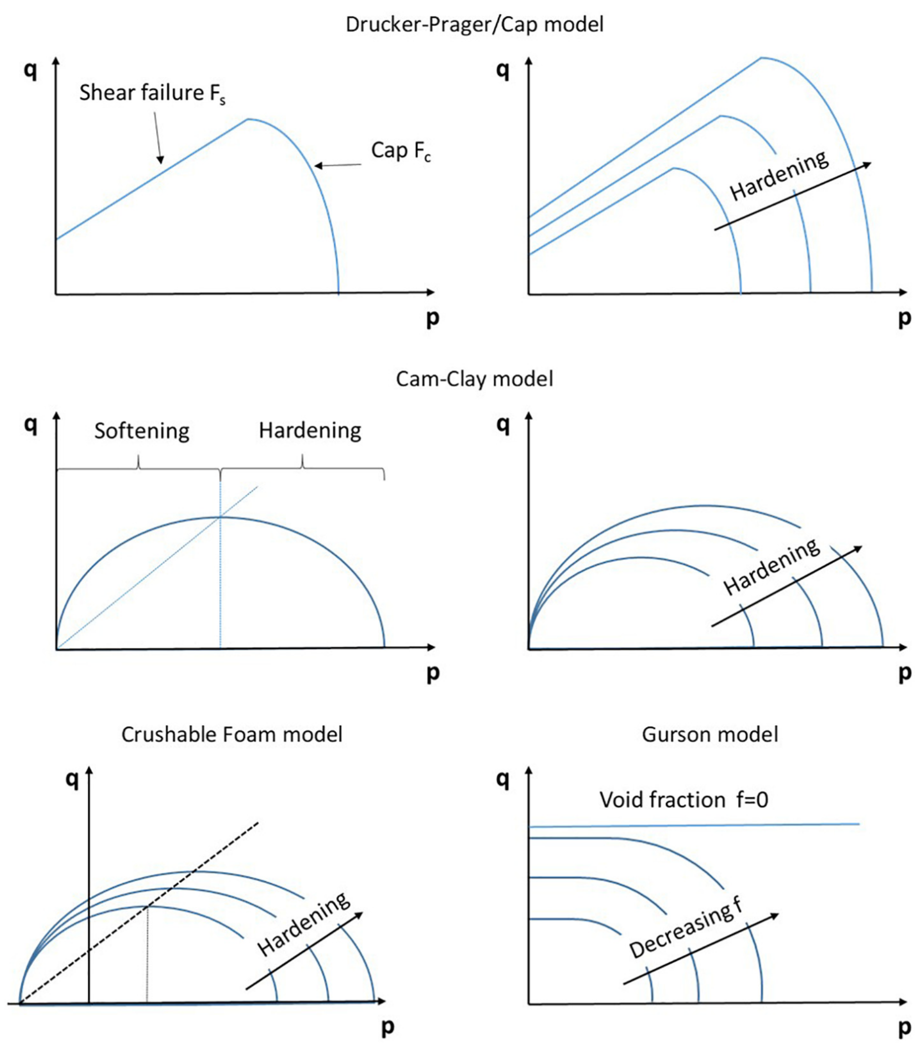

Fig. 1. Schematic of the Drucker-Prager/Cap model and the modified Cam-Clay model in the p-q plane. In addition to the shape of the yield surface the evolution of the yield surface with relative density (hardening) is shown. For powders with substantial tensile strength the yield surface for crushable foam and the Gurson yield surface for porous metal can be used.