Constitutive Model Development for Powder Compaction and Implementation into Abaqus

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Abstract: Die compaction of powders is a process which involves filling a die with powder, compaction using rigid punches to form a dense compact and ejection from the die. The process can be treated as a large deformation plasticity problem. The challenge is to develop and implement appropriate constitutive models that capture the evolution of the powder from a loose state into a dense compact. We present two practical modelling approaches using Abaqus:

1. *a modified Drucker-Prager cap model whereby all material parameters are described using density as state variable. The elastic properties are also expressed as a function of density.*

2. *a deformation plasticity model (for compaction only), focussing on a constitutive model valid for a specific class of powder materials that exhibits self similar loading surfaces during compaction. The model is implemented using the UHYPER or UMAT facility.*

We illustrate the applicability of the models to predict density distributions in powder compacts and discuss strategies for development of efficient computational schemes for powder compaction modelling.

Keywords: powder compaction, incremental plasticity, deformation plasticity, UHYPER, UMAT

1. Introduction

Die compaction of powders is used in powder metallurgy, ceramics, detergents, pharmaceutical tablets, nuclear fuel and other industries. Of practical interest is the manufacturing of compacts that are uniform (or have a defined internal density distribution) and crack free. The density variations in powder compacts result from a combination of the following five factors:

1. constitutive model

2. friction behaviour between powder and tooling (die and punches)

3. geometry of die and punches

4. loading schedule (sequence of punch motions)

5. initial conditions, which relate to the state of the powder after die fill

In this paper we focus on constitutive model development and implementation into Abaqus and present examples to illustrate how the density distribution is influenced by all factors listed above.

The paper is organised in 3 main parts. In Section 2 we discuss a modified Drucker-Prager cap model developed by Sinka et al. (2003). In section 3 we present an incremental plasticity framework developed by Cocks and Sinka (2007) and we discuss the development and implementation of a simplified deformation plasticity model (Sinka and Cocks, to appear). In Section 3 we discuss implementation into Abaqus using UHYPER and UMAT subroutines and illustrate the application of the model using an example. We conclude with general remarks on the development of efficient computational schemes for powder compaction modelling.

2. Established incremental plasticity modelling of powder compaction

Powder compaction can be treated as a finite deformation plasticity problem where the material properties evolve from a state characteristic to loose powders to one of a dense material. Thus, as a minimum, a yield surface and a hardening rule are needed. Powders can also be regarded as granular and porous materials, the behaviour of which is similar to rocks and soils. Therefore, not surprisingly, models adapted from the rock and soil mechanics literature have been adapted for powder compaction. Unlike fully dense metals, the yield behaviour of porous materials are different under tension and compression. In other words, the yield response depends on hydrostatic stress. One of the simplest models that capture this behaviour is the Drucker-Prager cap model (Drucker and Prager, 1952). A modified version of the model for powder compaction is presented in the next section.

2.1 A modified Drucker-Prager cap model

Consider a cylindrical powder specimen subjected to axial (σ_{ax}) and radial (σ_{rad}) stress as illustrated in Figure 1a. The yield surface is described by a shear failure line and a compaction surface, as illustrated in Figure 1b in the effective stress (σ_e) and hydrostatic stress (σ_m) space, where

$$\sigma_m = \frac{1}{3}\left(\sigma_{ax} + 2\sigma_{rad}\right) \tag{1}$$

$$\sigma_e = \sigma_{ax} - \sigma_{rad} \tag{2}$$

The shear failure line (Figure 1b) can be expressed as:

$$\sigma_e = c + \sigma_m \tan(\beta) \tag{3}$$

The shear failure line is defined by cohesion (c) and internal friction angle (β), which is determined using simple tests, such as uniaxial tension and compression, simple shear and diametrical compression. The compaction (cap) surface is described using an ellipse which is described by 2 parameters, therefore it requires 2 points in stress space, which can be obtained using various types of triaxial tests as illustrated in Figure 1 but also from the use of a die with radial stress measurement capability. In general the flow rule is taken associated for the compaction surface and non-associated along the shear failure line. This is important to capture the dilation of granular materials under shear.

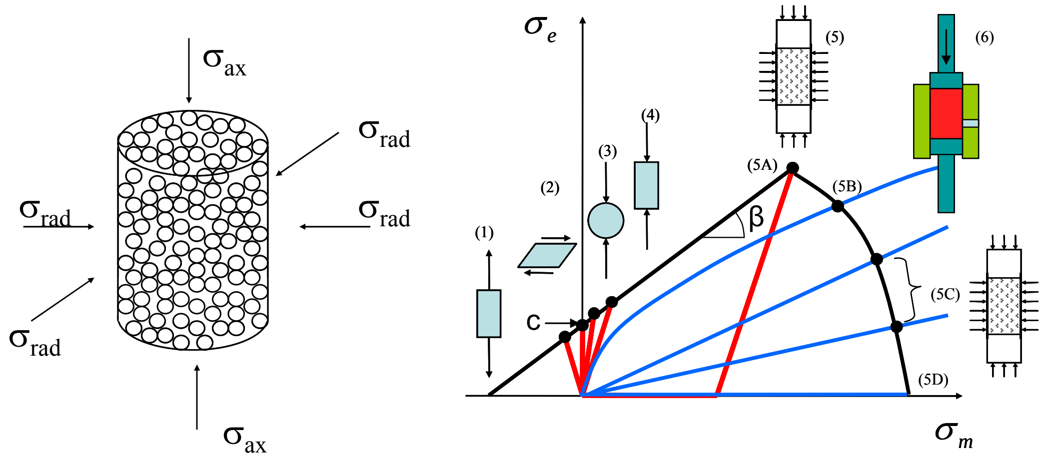


Figure 1: Constitutive models for powder compaction, a) stress measures, b) experimental procedures for determining Drucker-Prager cap model parameters. Failure line: (1) uniaxial tension, (2) simple shear, (3) diametrical compression, (4) uniaxial compression. Compaction surface: (5) triaxial testing: 5A consolidated triaxial test, 5B simulated closed die compaction, 5C radial loading in stress space, 5D isostatic test; (6) instrumented die compaction.

During compaction the material evolves from a loose state of powder into a dense compact. As presented elsewhere (Sinka et al., 2003) at every stage of the densification one can determine a Drucker-Prager type yield surface. Families of yield surfaces are presented in Figure 2, for microcrystalline cellulose powder, which is widely used in pharmaceutical tablet compaction. In effect this model uses relative density as state variable. Relative density is defined as the ratio between the density of the porous material and the density of the fully dense material.

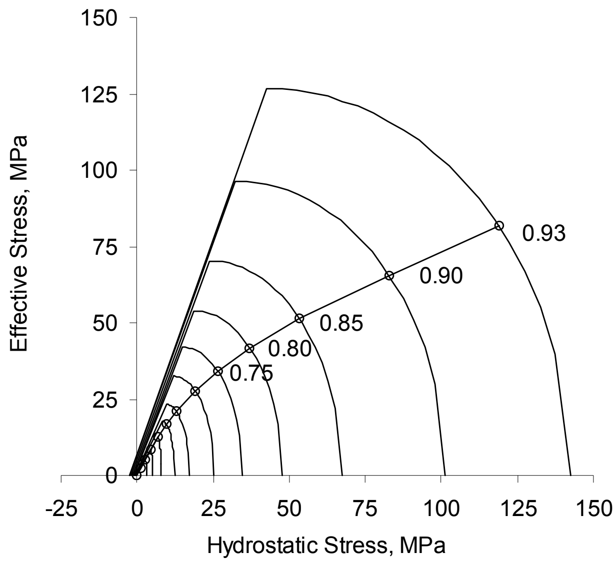
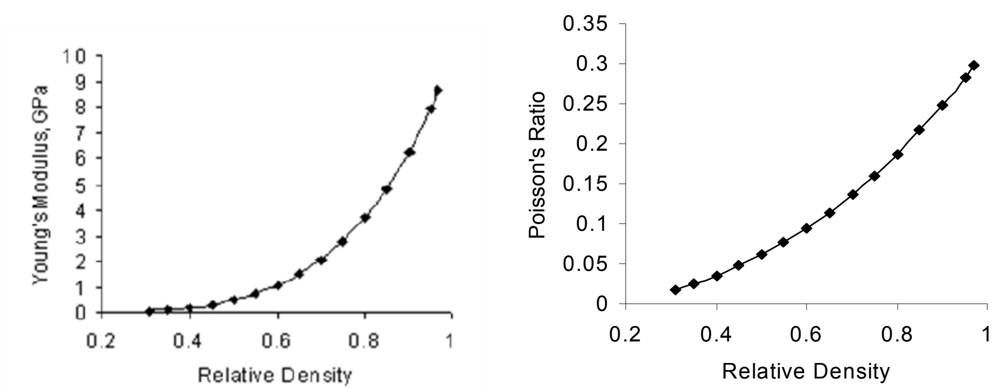


Figure 2 families of Drucker-Prager yield surfaces. The labels indicate relative density. The stress path corresponding to closed die compaction is also indicated (Sinka et al., 2003).

The elastic response can also characterised by performing tests on powder compacts pressed to different relative densities. A simple model, whereby the evolution of Young's modulus and Poisson's ratio is expressed as functions of relative density is illustrated in Figure 3.



(a) b)

Figure 3: Elastic parameters as functions of relative density. a) Young's modulus, b) Poisson's ratio (Sinka et al., 2003).

2.2 Friction between powder and die wall

The friction coefficient between powder and die wall can also be measured using a die instrumented with radial stress sensors. For consistency with the Section 2, we tested microcrystalline cellulose and it was found that the friction coefficient was dependent on contact pressure. Starting from high values at the early stages of compaction, the friction coefficient asymptotes to a lower value as the contact pressure (and density) is increased. Figure 4 illustrates the variation of friction coefficient for two cases:

1. clean die wall condition, where the die wall is degreased prior to compaction,
2. lubricated die wall condition, where a tablet of pure lubricant powder (magnesium stearate) is compressed prior to the experiment.

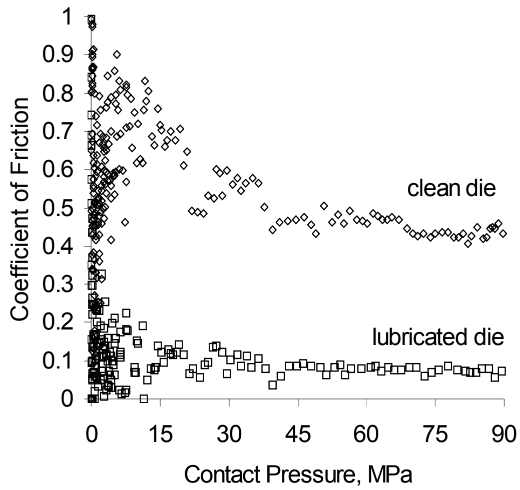
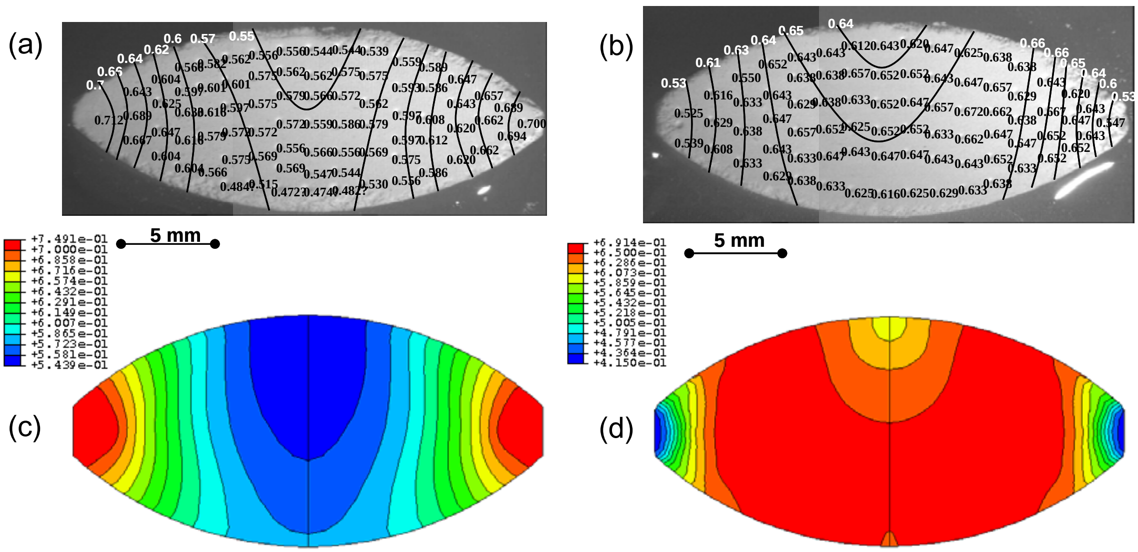


Figure 4: Coefficient of friction between powder and die wall.

Details on the data analysis procedures as well as a set of parametric studies on the importance of variable friction are presented elsewhere (Sinka et al. 2001). The relevance of high and low friction between powder and die wall (and powder and punches) is illustrated in the following section.

2.3 Density distribution in tablets made of pharmaceutical excipients

The modified Drucker-Prager cap model can readily be implemented in Abaqus standard. The contact pressure dependent friction coefficient can also be readily implemented in Abaqus, and other dependencies can also be included by employing the UFRIC facility. It is then possible to carry out simulations of the compression process using realistic material data. The density distribution in 2 convex faced tablets is presented in Figure 5 together with experimental validation of the results.



Clean (unlubricated) die and punches

Lubricated die and punches

Figure 5: Relative density distribution in 25mm diameter curved faced tablets. Experimental data for tablet compressed using a) clean and b) lubricated tooling. Numerical results for c) high and d) low friction (Sinka et al., 2003).

The only difference between the 2 simulations is the friction coefficient, which corresponded to clean and pre-lubricated die configurations as described in Section 5. Figure 5 illustrates that it is possible to make two identical tablets in terms of shape, weight and material which have different microstructures depending on the friction conditions employed. This has significant practical implications which are discussed elsewhere (Sinka et al., 2004).

In practice, incremental plasticity models such as described above, which use density or relative density as state variable are employed almost exclusively (PM Modnet Group, 2002). An alternative approach is described in the following section.

3. Deformation plasticity framework for powder compaction

The incremental plasticity approach is relatively complex, and even the simplest constitutive models have a significant number of material parameters that require calibration as functions of material state (usually described using density). In this section we describe a simple, deformation plasticity, approach noting that is valid for modelling the compaction step only.

3.1 Theoretical basis

The incremental plasticity framework is based on the existence of a yield surface and a flow rule. The empirical Drucker-Prager cap model assumes prescribed yield surfaces, which are not critically assessed. Cocks (Cocks, 2001; Cocks and Sinka, 2007) examined whether it was possible to develop a simple, single state variable model that captured the material behaviour for loading histories experienced in practical die compaction operations. For such loading histories it was found appropriate to consider a deformation plasticity model where the material behaviour is described using a potential function expressed in terms of the Kirchhoff stress. The strains can then be determined by differentiating the potential with respect to stress. The simplicity of the deformation plasticity model allows practical die compaction processes to be analysed in a computationally efficient manner.

Triaxial tests were conducted to validate the model for commercial metal powders (Sinka and Cocks, 2007). Figure 6 illustrates that it was possible to construct a consistent set of contours of constant complementary work done along radial loading paths in stress space.

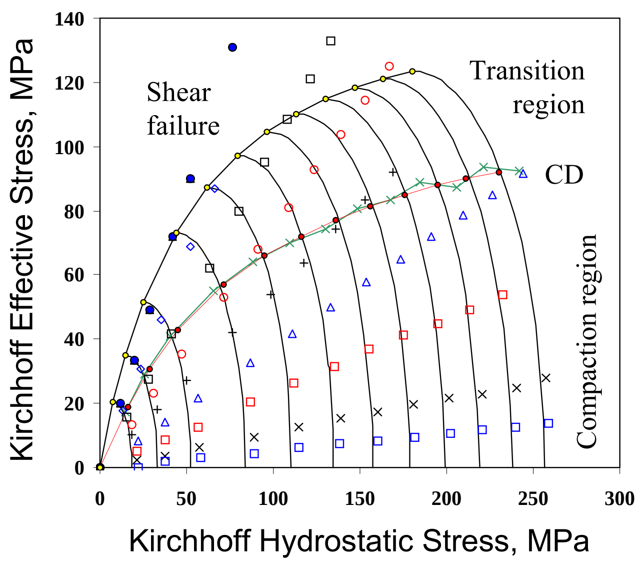


Figure 6: Contours of constant complementary work done (MJm^{-3}) per unit initial volume in Kirchhoff stress space. The data points represent stress states along radial loading paths in stress space and closed die compaction, labelled CD (Sinka and Cocks, 2007).

3.2 Development of a simplified deformation plasticity model

Once a consistent set of contours of complementary work done were developed, the next step is to establish a suitable form of the complementary work function that describes the surfaces. It is important to note that the stress path under closed die compaction for microcrystalline cellulose (see Figure 2) and the metal powder (see Figure 6) is a curve, indicating that the contours are not self similar geometrically.

Ceramic materials, however, present a particular behaviour in that the radial to axial stress ratio during die compaction is constant, which result in a radial loading stress path in the effective stress (σ_e) and hydrostatic stress (σ_m) space. Experimental data for calcium phosphate (a pharmaceutical powder) are presented in Figure 7 in a form suitable for further constitutive model development.

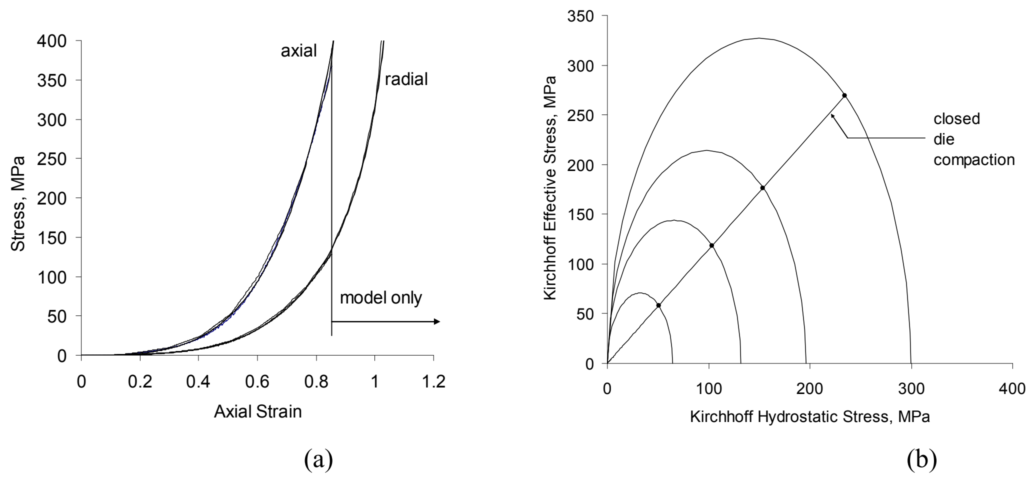


Figure 7: Experimental data and model calibration for calcium phosphate; a) radial and axial stress – axial strain, b) contours of constant complementary work done (Sinka and Cocks, to appear).

The deformation plasticity model developed by Cocks and Sinka (2007) is based on the construction of surfaces of constant complementary work in Kirchhoff stress space. A hyperelastic material can be defined where the total logarithmic strain E_{ij} is determined from a complementary energy function $\overline{\Omega}_e$, which is a function of the Kirchhoff stresses, T_{ij}

$$E_{ij} = \frac{\partial \overline{\Omega}_e}{\partial T_{ij}} \tag{4}$$

A dual potential, Ω_e also exists, which is a function of E_{ij}, such that

$$T_{ij} = \frac{\partial \Omega_e}{\partial E_{ij}} \tag{5}$$

and

$$T_{ij} E_{ij} = \overline{\Omega}_e + \Omega_e \tag{6}$$

When undertaking computational studies it is more convenient to express the response in terms of the strains E_{ij} and the potential Ω_e. Based on micromechanical considerations (Cocks and Sinka, 2007) during the early stages of compaction Ω_e is a quadratic function of the effective strain measure $\overline{E}$. The simplest form of potential function that satisfies the above requirements is:

$$\Omega_e = \frac{1}{2} A\overline{E}^2 + \frac{B\overline{E}^{\beta}}{\left(E_v^{\max} - \overline{E}\right)^{\alpha}} \tag{7}$$

In the limit of small strains the quadratic term dominates if $\beta > 2$. The second term dominates during the later changes of compaction, and the volumetric strain can never exceed the limit $E_v^{\max}$, which corresponds to full density. The effective strain $\overline{E}$ is defined in Sinka and Cocks (to appear). The model (Equation 7) can now be calibrated based on the experimental data.

4. Model implementation in Abaqus using UHYPER and UMAT

The strain energy functions currently available in Abaqus for incompressible or highly compressible elastic materials do not offer the flexibility for implementing the particular form described by Equation (7). However, an arbitrary strain energy potential function can be defined using the UHYPER facility to model isotropic hyperelastic material behaviour. Alternatively, an arbitrary constitutive model can be implemented using the UMAT user defined material subroutine.

In UHYPER, a strain energy function Ω_e is defined as a function of invariants of the deviatoric stretch tensors $\overline{I_1}$, $\overline{I_2}$ and the deformation Jacobian *J*. The strain E_e can be expressed as a function of $\overline{I_1}$ and $\overline{I_2}$ and $E_v = -\ln J$ (which we define, for convenience, as being positive in compression). Therefore

$$\Omega_e = \Omega_e\left(\overline{I_1}, \overline{I_2}, J\right) = \Omega_e(E_e, E_v) \tag{8}$$

UHYPER also requires the first, second and third order derivatives of Ω_e with respect to $\overline{I_1}$, $\overline{I_2}$ and *J* to be defined.

Using Equations (7) and (8), it is possible to determine analytically all the required derivatives of $\overline{I_1}$, $\overline{I_2}$ and *J*. It is useful to note that in our model the potential function and its derivatives are expressed as functions of the deviatoric principal stretches. This provides a more general framework, however, the principal stretches could not readily be passed into UHYPER. To overcome this problem we defined the deviatoric principal stretches as state variables, which could then be accessed in UHYPER.

4.1 Density distribution in cylindrical components using deformation plasticity

Another example of ceramic powder material that exhibits self similar loading surfaces for which the simplified deformation plasticity model applies is alumina powder. The compaction of a 30mm OD, 10 mm ID alumina ring is examined here. The tooling is composed of a die, a central rod and upper and lower punches, which are modelled as rigid surfaces. For this geometry any density variations come about from the friction interaction between powder and tooling (we used a friction coefficient of 0.1 for all contact surfaces) and the pressing sequence (here the lower punch was prescribed stationary) as the initial relative density (0.35) was assumed constant.

Snapshots of the evolution of internal density distribution during compaction are presented in Figure 8 in a vertical cross-section of the compact. Density variations in powder compacts are important as they influence the local mechanical properties (i.e. post-compaction behaviour) and shrinkage behaviour during sintering.

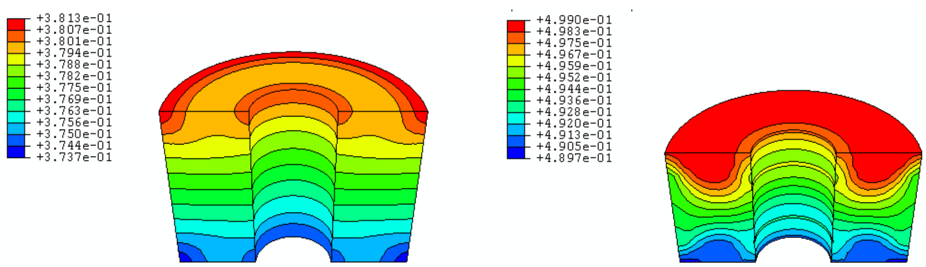


Figure 8: Relative density distribution in a powder pressed ring at various stages during compaction.

5. Concluding remarks

In this paper we presented a summary of incremental and deformation plasticity models developed for powder compaction and detailed the implementation of the deformation plasticity model into Abaqus. The models were developed and calibrated using carefully conducted experiments. We discussed particular features of the behaviour of a range of powder materials such as metallic powders, polymers and ceramics. Appropriate models were developed with emphasise on simplicity, relevance and applicability to practical powder compaction processes.

The deformation model is efficient for modelling compaction however, it does not capture the material response during unloading, ejection and post-compaction operations, which require a detailed knowledge of the actual yield surfaces. To model unloading and ejection, it is necessary to change to an incremental plasticity framework, in which the form of the yield surface at the end of compaction is determined from the plastic state determined from the deformation plasticity model. Full coupling of the two models is subject to ongoing research.

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