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AN EULERIAN APPROACH FOR DIE COMPACTION PROCESSES

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SUMMARY
For the analysis of deformation processes the Eulerian approach is usually formulated in material velocities. To describe the die compaction of compressible media, this paper presents an Eulerian simulation method, basically expressed in displacements. The material behaviour is modelled by the theory of elastoplasticity. Frictional interaction with the surroundings is included. As a spatially fixed finite element mesh is applied, rezoning is governed by the process specification and not, as in the Lagrangian approach, by the mesh distortion. The solution scheme, using a Newton–Raphson algorithm, is considered in detail. A consistent iteration procedure is derived. Examples demonstrate the merits of the method developed.

1. INTRODUCTION
The die compaction of granular materials can be considered as a particular stage in manufacturing many ceramic products. To ensure product quality it is desired that after pressing the density of the so-called 'green' compact is 'as homogeneous as possible', while the level of residual stresses is 'sufficiently low'. The distribution of the density and the stress state are determined by the constitutive behaviour of the powder material and by the external friction (interaction between the powder and the punch/die wall). The specification, quantification and validation of constitutive models from experimental research still constitute a delicate problem.

The aim of this paper is to present an Eulerian simulation method formulated in material displacements. This offers advantages over the usual approaches when it is necessary to account for material flow around (non-smooth) corners. Besides, attention will be given to a consistent iterative solution algorithm.

During powder compaction in a die ('pressing to size'), the internal volume between punch and die is monotonically reduced, prescribed by the punch displacement as a function of the time. To ensure product quality it is necessary that, apart from the very initial stages of compaction processes, the internal volume remains completely filled with powder material without the occurrence of cavities. To take account of this feature, it is supposed that for any time \( t \) in the total compaction range of time, the volume \( V_t \) occupied by powder material is exactly known in advance. Unloading of pressed compacts will not be considered.

For the characterization of the granular material deformation a continuum mechanics approach will be followed. The point of departure is the local existence of the deformation gradient tensor \( \mathbf{F} \), related to an appropriate reference state. For a current state this tensor is defined by the
\[ dx = F \cdot dx, \]  

where \( dx \) is an arbitrary, infinitesimally small vector between two material points in the reference state and \( dx \) the associated (material) vector in the current state. As viscous and thermal effects are neglected, the tensor \( F \) and its history determine the local Cauchy stress tensor \( \sigma \).

It is assumed that the process conditions allow for a quasistationary approach where a number of subsequent equilibrium states is examined. The time variable \( \tau \) should be considered as a monotonically increasing parameter, introduced to indicate the level of progress in the deformation process only. The mathematical modelling for a particular process stage at the time \( \tau \) leads to the following requirements:

(i) the stress tensor field should satisfy the local equilibrium equations for any point in \( V \);
(ii) the stress tensor should be related to the local deformation and the deformation history by the constitutive equation (to be specified) for the continuum material at any point in \( V \);
(iii) the kinematical and dynamical boundary conditions should be satisfied in conformity with the global process specification (\( V \) is prescribed) and with the constitutive equation for the contact phenomena (friction) occurring due to interaction between the powder material and the punch/die material; stick/slip will be governed by Coulomb's law.

For relevant practical problems, results can be obtained exclusively with the application of numerical methods. In general, compaction simulation examples in the literature are confined to finite element approximations, based on a Lagrangian problem formulation. The element geometry changes are determined by the deformation of the powder material. Initially 'well-shaped' elements can become unacceptably distorted during the process, inducing theoretical and numerical problems. The calculation for slip along non-smooth boundary parts (space-associated conditions) is intrinsically involved with kinematical inaccuracies. By the application of rezoning the difficulties can be surmounted; however, the procedure generally requires manual interference, which is an obstacle to a fully self-controlled computational process simulation.

This paper deals with the simulation of compaction processes, based on an elaboration of the Eulerian problem description with the finite element method. A physical quantity is considered to be a function of the time \( \tau \) and of the position vector \( x \) in the geometrical space. For the present research the relevant domain \( V \) of \( x \) is dependent on the time \( \tau \). The particular material particle with position vector \( x \) at time \( \tau \) can be formally identified by \( x, = x, (x, \tau) \). For the actual displacement \( u(x, \tau) \) of that particle with respect to the reference state it holds that

\[ u(x, \tau) = x - x,(x, \tau) \]  

The calculation for space-associated boundary conditions can be performed easily, which is definitely the motive here for the application to die compaction processes. As the finite elements are fixed in space, the typical disadvantages of the Lagrangian approach as a consequence of kinematical incompatibility along the boundary are avoided. Finite element meshes for subsequent stages (\( \tau = t \) and \( \tau = t + \Delta t \)) of the compaction process differ because of changing boundary geometry (\( V \) decreases to \( V_{t+\Delta t} \)). The adaptations, however, can be specified in advance as it is supposed that \( V \) is a priori known as a function of the time \( \tau \). Actually the element mesh for \( \tau = t + \Delta t \) is obtained from the mesh for \( \tau = t \) by local reduction or removal of elements.

The strategy, developed to solve numerically the differential problem formulation and boundary conditions with application of the Eulerian approach, is explained in Section 2. A number of subsequent stages in the compaction process, which are defined by prescribed finite time steps (increments), is considered. For each stage the discretized equilibrium equations are derived,
based on the finite element method. The substitution of the constitutive continuum relationships into these equations results in the non-linear system

$$\mathbf{f}_i(\mathbf{u}) = \mathbf{f}_e$$

with $\mathbf{f}_i$ and $\mathbf{f}_e$ columns with internal and external nodal forces, respectively, and with $\mathbf{u}$ the column with incremental nodal displacements. When the boundary conditions are included, the system (3) can be solved formally. For the actual solution the iterative Newton-Raphson scheme is applied. Preparatory calculations are performed for that purpose. In Section 3 attention is focussed on the mechanical behaviour of granular materials. It is common practice to adopt the concepts of the theory of elastoplasticity, leading to a rate formulation of the constitutive equation. The integration is discussed and iterative relationships are derived. From the wide variety of models in the literature, a simple model is selected for further elaborations. In Section 4 the material model is quantified. For a number of compaction processes the results of the numerical simulation are presented.

2. COMPUTATIONAL STRATEGY

An incremental analysis procedure\(^1\) is executed with calculations for a discrete number of subsequent load levels at specific times. In this section the foundations of the incremental calculations are explained by focussing on a single step $t \leq \tau \leq t + \Delta t$. It is supposed that at the beginning of the increment ($\tau = t$) the distribution of the Cauchy stress components in the domain $V_t$ is known: the stress tensor field $\sigma(x)$ with the position vector $x$ in $V_t$ is explicitly specified. The local previous deformation history, represented by the column with so-called history parameters $\eta_t$, is also assumed to be available, implying the specification of $\eta_t(x)$ with $x$ in $V_t$. The size of the increment is defined by prescribing the geometry of the continuum boundary at the time $\tau = t + \Delta t$ enclosing $V_{t+\Delta t}$. The aim is to determine the state of the continuum at the end of the increment ($\tau = t + \Delta t$). This involves the calculation of the fields of the Cauchy stress tensor and the history parameters, $\sigma_t+\Delta t(x)$ and $\eta_t+\Delta t(x)$, respectively, for $x$ in the domain $V_{t+\Delta t}$. Through discretization the incremental transition is described by a non-linear set of (algebraic) equations. The final solution is obtained using an iterative scheme.

The incremental displacement $\mathbf{u}(x)$ for a material point $P$ is visualized in Figure 1. For points with a position vector $x$ on the boundary of $V_{t+\Delta t}$ the vector $x - \mathbf{u}(x)$ should end on the boundary of $V_t$. The local deformation of the continuum is described by the deformation gradient tensor $\mathbf{F}$, see (1), here defined with respect to the configuration at the start of the increment. For a particle with position vector $x$ at time $\tau = t + \Delta t$, it is easily shown that

$$\mathbf{F}(x) = [\mathbf{I} - \nabla \mathbf{u}]^{-c}$$

Figure 1. Incremental displacement
with \( \mathbf{I} \) being the second-order unit tensor and \( \nabla \) the gradient operator in the current configuration \( V_{t+\Delta t} \). The superscript \( c \) denotes conjugation. At the start of the increment the stress tensor and the history parameters for the particle are given by \( \mathbf{\sigma}_t(x - \mathbf{u}(x)) \) and \( \mathbf{\eta}_t(x - \mathbf{u}(x)) \), respectively. The stress tensor and the history parameters at \( \tau = t + \Delta t \), \( \mathbf{\sigma}_{t+\Delta t}(x) \) and \( \mathbf{\eta}_{t+\Delta t}(x) \), can be determined if \( \mathbf{u}(x) \) and \( \mathbf{F}(x) \) are given and if additional assumptions with respect to the deformation path, to be presented in the next section, are made. The stress field \( \mathbf{\sigma}_{t+\Delta t}(x) \) with \( x \) in \( V_{t+\Delta t} \), expressible in the incremental displacement field as indicated, has to obey the local equilibrium equation.

To manipulate the differential problem formulation, the incremental displacement field \( \mathbf{u}(x) \) with \( x \) in \( V_{t+\Delta t} \) is approximated by a finite element discretization

\[
\mathbf{u}(x) = \mathbf{N}^T(x)\mathbf{u}
\]

(5)

The nodal displacement vectors constitute the column \( \mathbf{u} \), the column \( \mathbf{N}(x) \) contains the set interpolation functions. The superscript \( T \) denotes transposition. For an element \( e \) the displacement interpolation can be written analogous to (5), so

\[
\mathbf{u}(x) = \mathbf{N}^e(x)\mathbf{u}^e
\]

(6)

with \( \mathbf{u}^e \) the element nodal displacement vector column and with \( \mathbf{N}^e(x) \) containing the elemental shape functions.

As pointed out earlier, the stress field \( \mathbf{\sigma}_{t+\Delta t}(x) \) and the field of history parameters \( \mathbf{\eta}_{t+\Delta t}(x) \) can be expressed in the displacement field and therefore, using (5), in the column \( \mathbf{u} \). This column must be determined such that the stresses obey the discretized\(^6\) equilibrium equation

\[
\mathbf{f}_i(\mathbf{u}) = \mathbf{f}_e
\]

(7)

where the columns with internal and external nodal forces are defined by

\[
\mathbf{f}_i(\mathbf{u}) = \int_{V_{t+\Delta t}} [\nabla \mathbf{N}] \cdot \mathbf{\sigma}_{t+\Delta t} \, dV
\]

(8)

\[
\mathbf{f}_e = \int_{A_{t+\Delta t}} \mathbf{N} \cdot \mathbf{p}_{t+\Delta t} \, dA
\]

(9)

with \( \mathbf{p}_{t+\Delta t} \) the stress vector acting on the boundary \( A_{t+\Delta t} \). For nodal points inside the boundary of the element mesh the components of \( \mathbf{f}_i \) are equal to zero, for nodes on the boundary of the mesh the boundary conditions have to be taken into account. The column \( \mathbf{f}_i(\mathbf{u}) \) is completely determined by the stress distribution \( \mathbf{\sigma}_{t+\Delta t}(x) \) and consequently by the nodal displacements \( \mathbf{u} \), as was outlined previously.

The calculation of internal nodal forces with equation (8) will be performed numerically using Gaussian integration points. Then for the total assemblage of elements it can be written that

\[
\mathbf{f}_i(\mathbf{u}) = \sum_{p \in \mathcal{I}_p} \mathbf{v}^p [(\nabla \mathbf{N})^p] \cdot \mathbf{\sigma}^p_{t+\Delta t}
\]

(10)

where the superscript \( p \) indicates a particular integration point with position vector \( x^p \) and \( \mathcal{I}_p \) is the total set of integration points for all continuum elements at time \( \tau = t + \Delta t \). The quantity \( \mathbf{v}^p \) denotes the volume fraction associated with integration point \( p \). For the elaboration of (10) the stress tensor \( \mathbf{\sigma}^p_{t+\Delta t} = \mathbf{\sigma}_{t+\Delta t}(x^p) \) in the integration points has to be determined. This requires the availability of \( \mathbf{\sigma}_t(x^p - \mathbf{u}(x^p)) \), \( \mathbf{\eta}_t(x^p - \mathbf{u}(x^p)) \) and \( \mathbf{F}(x^p) \). As \( \mathbf{u}(x^p) \) and \( \mathbf{F}(x^p) \) for an integration point \( p \) in element \( e \) can be expressed in the element nodal displacements \( \mathbf{u}^e \), it is possible to compute the contribution of that element to the column \( \mathbf{f}_i \), the internal element nodal forces,
when the column $u^*$ is known. With a standard organization scheme the element contributions are assembled to build up the column $f_i$.

For an arbitrary integration point in the continuum with position vector $x^p$ at time $\tau = t + \Delta t$, the stress tensor $\sigma^R_{t + \Delta t} = \sigma_{t + \Delta t}(x^p)$ and the history parameters $\eta^R_{t + \Delta t} = \eta_{t + \Delta t}(x^p)$ are to be determined from the constitutive equations. Section 3 deals specifically with the particular constitutive formulation for the continuum material and presents further elaborations. It is preferred, however, to discuss here the calculation of the relevant quantities and to pay attention to the structure of the final mathematical form following from the constitutive modelling.

At the start of the present increment, which describes the transition of the material during the range $t \leq \tau \leq t + \Delta t$, it is supposed that the numerical results for $\sigma_i(x)$ and $\eta_i(x)$ at the end of the previous increment are available as (averaged) discrete quantities in the nodal points of the element mesh for that increment. To determine the value of $\sigma_i$ and $\eta_i$ for $x = x^p - u(x^p)$ formally a laborious search method in the mesh for the volume $V_i$ has to be applied. To avoid that, an alternative approach is proposed in this paper to express $\sigma_i(x)$ and $\eta_i(x)$ in $u$. Based on interpolation techniques $\sigma_i(x)$ and $\eta_i(x)$ are calculated in the nodes of the actual mesh for $V_{t + \Delta t}$. The nodal results are contained in the column $\sigma_i$ and the matrix $\eta_i$ (each row in $\eta_i$ equals $\eta_i^T$ for the associated nodal point), ordered analogous to $u$ in equation (5). It is noted that the interpolation can be omitted if the actual nodes in $V_{t + \Delta t}$ coincide with the nodes in the previous mesh for $V_t$.

The tensor column $\sigma_i$ and the matrix $\eta_i$ are used for a modified discretization of the fields $\sigma_i(x)$ and $\eta_i(x)$. In conformity with (5) this can be written as

$$\sigma_i(x) = N^T(x) \sigma_i = \sigma_i^T N(x)$$

(11)

$$\eta_i(x) = [N^T(x) \eta_i]^T = \eta_i^T N(x)$$

(12)

only defined and applicable for $x$ in the domain $V_{t + \Delta t}$. With these expressions and using (5) it can be derived that approximately

$$\sigma_p^p = \sigma_i(x^p) - u(x^p) \cdot (\nabla \sigma_i)^p = \sigma_i^T [I - \nabla N]^p \cdot u^T N(x^p)$$

(13)

$$\eta_p^p = \eta_i(x^p) - u(x^p) \cdot (\nabla \eta_i)^p = \eta_i^T [I - (\nabla N)^p \cdot u^T] N(x^p)$$

(14)

The deformation gradient tensor $F^p$ in an integration point can be derived immediately after substitution of equation (5) into (4):

$$F^p = [I - ((\nabla N)^p)^T u]^{-e}$$

(15)

The formulas (13), (14) and (15) provide the constitutive input variables, expressed in the incremental displacements of the nodal points. It should be realized that the procedure outlined above enables an elaboration of (10) at element level. The elemental contribution to the internal nodal forces column $f_i$ can be determined exclusively with the particular components of $u_i$, $\sigma_i$, and $\eta_i$ for the element nodes. To explain further elaborations some attention is given to the computation of the stress tensor $\sigma^R_{t + \Delta t}$ for an integration point $p$ at the time $\tau = t + \Delta t$. Advancing on Section 3 it is stated that the final constitutive formulation will read

$$\sigma^R_{t + \Delta t} = R^p \cdot [\sigma^p + \Delta \sigma^p] \cdot [R^p]^c$$

(16)

where $R^p$ is the rotation tensor following from polar decomposition of the deformation gradient tensor $F^p$. The tensor $\Delta \sigma^p$ denotes the rotation-neutralized incremental change of the Cauchy stress tensor, formally to be expressed as

$$\Delta \sigma^p = \hat{\sigma}^R_p (\sigma^p, \eta^p, e^p) : e^p$$

(17)
where $4\hat{\mathbf{M}}_i = 4\hat{\mathbf{M}}_i(\mathbf{s}_i, \eta_i, \mathbf{e})$ is the rotation-neutralized averaged fourth-order constitutive tensor and $\mathbf{e}^p$ the logarithmic strain tensor defined by

$$\mathbf{e}^p = \frac{1}{2} \ln \left( \left[ [\mathbf{F}^p]^{-1} \cdot \mathbf{F}^p \right] \right)$$

(18)

The global structure of the constitutive formulation is needed in order to explain the numerical elaboration and the iterative relationships in the sequel.

For an arbitrary continuum element $e$ the contribution $f_{f_i}^e$ to the column $f_i$ of internal nodal forces can be expressed in the nodal quantities $\mathbf{u}^e$, $\mathbf{s}_i^e$ and $\eta_i^e$ for that element, constituting the relevant partitions from the global quantities $\mathbf{u}$, $\mathbf{s}_i$ and $\eta_i$, respectively. For integration point $p$ of element $e$ the equations (13), (14) and (15) are

$$\sigma_i^e = \mathbf{s}_i^e T \left[ \mathbf{I} - (\mathbf{V}^N)^p \cdot \mathbf{u}^e T \right] N_i^e(x^p)$$

(19)

$$\eta_i^e = \eta_i^e T \left[ \mathbf{I} - (\mathbf{V}^N)^p \cdot \mathbf{u}^e T \right] N_i^e(x^p)$$

(20)

$$\mathbf{F}^p = \left( \mathbf{I} - \left( \mathbf{V}^N \right)^p \right)^T \left[ \mathbf{u}^e \right]^{-1}$$

(21)

Based on $\sigma_i^e$, $\eta_i^e$ and $\mathbf{F}^p$, the stress tensor $\sigma_i^{e,\Delta}$ can be calculated. When the set of integration points for element $e$ is denoted by $\mathcal{P}_i$, for the element column $f_i^e = f_i^e(\mathbf{u}^e)$ it holds, in conformity with (10), that

$$f_i^e(\mathbf{u}^e) = \sum_{p \in \mathcal{P}_i} \mathbf{v}^p \left( (\mathbf{V}^N)^p \right) \cdot \sigma_i^{p,\Delta}$$

(22)

It is obvious that (22) represents the element internal nodal forces $f_i^e$, expressed in the element nodal displacements $\mathbf{u}^e$ through a complicated non-linear relationship. The non-linearity at element level propagates to the system equations (7) and necessitates an iterative solution scheme. The standard Newton–Raphson method is applied, requiring the consistent relationships between (infinitesimally) small changes of $\Delta \mathbf{u}$ and the associated changes of $f_i^e$ at element level:

$$\delta f_i^e = \dot{\mathbf{Q}}^e \cdot \delta \mathbf{u}^e; \quad \dot{\mathbf{Q}}^e = \left\{ \begin{array}{c} \left( \frac{\delta \mathbf{F}}{\delta \mathbf{u}_i} \right)^e \vspace{1mm} \\
\left( \frac{\delta \mathbf{F}}{\delta \mathbf{u}_i} \right)^e \end{array} \right\}^T$$

(23)

where $\dot{\mathbf{u}}^e$ denotes an estimate for the displacement column $\dot{\mathbf{u}}^e$. The matrix $\dot{\mathbf{Q}}^e$, determined by the estimated state only, is called the elemental tangential stiffness matrix. Firstly, for the calculation of $\dot{\mathbf{Q}}^e$ the iterative change of $\Delta \sigma^p$, occurring in equation (16), is considered. With (17) the following is obtained:

$$\delta \Delta \sigma^p = 4\hat{\mathbf{M}}_i(\mathbf{s}_i^p, \eta_i^p, \mathbf{e}^p) : [\dot{\mathbf{e}}^p + \delta \mathbf{e}^p] - 4\hat{\mathbf{M}}_i(\mathbf{s}_i^p, \eta_i^p, \mathbf{e}^p) : \dot{\mathbf{e}}^p$$

(24)

It is assumed that only small disturbances in the iterative procedure are introduced when this equation is replaced by

$$\delta \Delta \sigma^p = 4\hat{\mathbf{M}}_i : \delta \mathbf{e}^p$$

(25)

with $4\hat{\mathbf{M}}_i = 4\hat{\mathbf{M}}_i(\mathbf{s}_i^p, \eta_i^p, \mathbf{e}^p)$ being the iterative rotation-neutralized fourth order constitutive tensor, defined such that

$$4\hat{\mathbf{M}}_i : \delta \mathbf{e}^p = 4\hat{\mathbf{M}}_i(\mathbf{s}_i^p, \eta_i^p, \mathbf{e}^p) : [\dot{\mathbf{e}}^p + \delta \mathbf{e}^p] - 4\hat{\mathbf{M}}_i(\mathbf{s}_i^p, \eta_i^p, \mathbf{e}^p) : \dot{\mathbf{e}}^p$$

(26)

holds for any small $\delta \mathbf{e}^p$. The construction of $4\hat{\mathbf{M}}$ will be considered in Section 3. Secondly, using (25), the iterative form of (16) reads

$$\delta \sigma_i^{p,\Delta} = \delta \mathbf{R}^p \cdot [\dot{\mathbf{R}}^p]^c \cdot \dot{\sigma}_i^{p,\Delta} + \dot{\sigma}_i^{p,\Delta} \cdot \dot{\mathbf{R}}^p \cdot [\delta \mathbf{R}^p]^c$$

$$+ \dot{\mathbf{R}}^p \cdot [\delta \sigma_i^p + 4\hat{\mathbf{M}}_i : \delta \mathbf{e}^p] \cdot [\dot{\mathbf{R}}^p]^c$$

(27)
As the iterative changes $\delta \mathbf{R}^p$, $\delta \mathbf{\sigma}^p$ and $\delta \mathbf{\varepsilon}^p$ can be expressed linearly in $\delta \mathbf{u}^e$, relationship (27) reads in concise notation

$$\delta \mathbf{\sigma}^p_{+A} = [\mathbf{3}^p][T] \cdot \delta \mathbf{u}^e$$

(28)

where $\mathbf{3}^p$ is a column which contains third-order tensors. Finally, substitution of (28) into the iterative version of (22) and comparison with (23) result in a formula for the elemental tangential stiffness matrix

$$\dot{\mathbf{Q}}^e = \sum_{p \in \mathcal{P}} \nu^p [\mathbf{V}^p] \cdot [\mathbf{3}^p]^T$$

(29)

which closes the manipulations at element level.

An assemblage process over the total number of elements yields the iterative formulation for the global column with internal nodal forces

$$\delta \mathbf{f}_i = \dot{\mathbf{Q}} \cdot \delta \mathbf{u}$$

(30)

with $\dot{\mathbf{Q}}$ being the global tangential stiffness matrix. The iterative expression that will be used to solve the system equations (7) reads

$$\dot{\mathbf{Q}} \cdot \delta \mathbf{u} = \mathbf{f}_e - \mathbf{f}_i(\mathbf{u})$$

(31)

The boundary conditions can be taken into account using straightforward procedures (e.g. Brekelmans3). Actually, friction elements have been introduced to obtain a suitable formulation.

3. CONSTITUTIVE EQUATIONS FOR GRANULAR MATERIALS

The constitutive modelling of the granular material behaviour is of fundamental importance for the simulation of powder compaction processes. Since viscous and thermal effects are excluded, the Cauchy stress tensor $\mathbf{\sigma}(t)$ for an actual time $t$ depends only on the deformation gradient tensor $\mathbf{F}$ and its history from a specified initial state. The relationship between $\mathbf{\sigma}(t)$ and the evolution of $\mathbf{F}(\tau)$, $\tau \leq t$ can be denoted formally with a functional expression. The general foundations applied in the theory of metal elastoplasticity are adopted to describe the behaviour of granular materials.15 This leads to a rate formulation which is more suitable than a functional one. Objectivity requirements result in

$$\dot{\mathbf{\sigma}} = \mathbf{\dot{\sigma}} - \Omega \cdot \mathbf{\sigma} - \mathbf{\sigma} \cdot \Omega^c = \mathbf{4M} : \mathbf{D}$$

(32)

where $\mathbf{\dot{\sigma}}$ is the (objective) Jaumann rate of the Cauchy stress tensor $\mathbf{\sigma}$ and $\mathbf{\dot{\sigma}}$ is the (non-objective) material time derivative of $\mathbf{\sigma}$. The spin tensor $\mathbf{\Omega}$ and the deformation rate tensor $\mathbf{D}$ are the skew-symmetric and the symmetric part of the product $\dot{\mathbf{F}} : \mathbf{F}^{-1}$, respectively. The constitutive tensor $\mathbf{4M}$ represents the instantaneous material properties. It can be shown that $\mathbf{4M}$ depends on the actual stress tensor $\mathbf{\sigma}$ and the actual values of the history parameters $\mathbf{\eta}$ (also called internal or hidden variables): $\mathbf{4M} = \mathbf{4M}(\mathbf{\sigma}, \mathbf{\eta})$. The evolution of the history parameters is formulated as

$$\dot{\mathbf{\eta}} = \mathbf{Y} : \mathbf{D}$$

(33)

with $\mathbf{Y} = \mathbf{Y}(\mathbf{\sigma}, \mathbf{\eta})$ being a column containing tensorial quantities. The equations (32) and (33) constitute a system of mutually coupled differential equations. In the sequel the simultaneous time integration of these equations is discussed to derive the expressions (16) and (17), while the iterative relationship (25) is also supported.

An incremental deformation process during a time step $\tau \leq t \leq t + \Delta t$ is considered. It is supposed that for the time $\tau = t$ the state is given by the stress tensor $\mathbf{\sigma}(t)$ and by the history
parameters \( \eta(t) \). The deformation process for the increment \( t \leq \tau \leq t + \Delta t \) is defined by the deformation gradient tensor \( F(t) \). The configuration for \( \tau = t \) is indicated as the reference for the deformation, so \( F(t) = I \) with \( I \) being the unit tensor. The integration of (32) and (33) should result in \( \sigma(t + \Delta t) \) and \( \eta(t + \Delta t) \) for the end of the increment. If only \( F(t + \Delta t) \) is supplied, as in the present research, assumptions with respect to the deformation path have to be added, in order to obtain a unique solution for \( \sigma(t + \Delta t) \) and \( \eta(t + \Delta t) \). It is possible to establish these assumptions in such a manner that with the integration process only rotation-neutralized quantities are involved.\(^{12} \) The rotational effects are then taken into account after the numerical integration. In this way it is achieved that the final solution obeys objectivity requirements. If it is assumed that during \( t \leq \tau \leq t + \Delta t \) the directions of the eigenvectors of the logarithmic strain tensor \( \varepsilon(\tau) \), defined as in (18), remain unchanged, it can be proved that

\[
\dot{\sigma} = R \cdot \dot{\sigma} \cdot R^c
\]  

(34)

with \( R = R(\tau) \) being the rotation tensor following from polar decomposition of \( F(\tau) \) and with \( \dot{\sigma} = \dot{\sigma}(\tau) \) the rotation-neutralized stress tensor, defined by

\[
\dot{\sigma}(\tau) = R^c(\tau) \cdot \sigma(\tau) \cdot R(\tau)
\]  

(35)

With the introduction of the rotation-neutralized deformation rate tensor \( \hat{D} = \hat{D}(\tau) \), defined analogously to \( \dot{\sigma} \) in (35), equation (32) transforms into

\[
\dot{\sigma} = \hat{\mathbf{M}} : \dot{\varepsilon}
\]  

(36)

where \( \hat{\mathbf{M}} = \hat{\mathbf{M}}(\dot{\sigma}, \eta) \) denotes the rotation-neutralized constitutive tensor. As the principal directions of the strain tensor \( \varepsilon \) are assumed to be constant during \( t \leq \tau \leq t + \Delta t \), the tensor \( \hat{D} \) equals \( \dot{\varepsilon} \). The final rate formulation for the constitutive behaviour reads

\[
\hat{\sigma} = \hat{\mathbf{M}} : \dot{\varepsilon}
\]  

(37)

while the hardening evolution (33) can similarly be transformed into

\[
\dot{\eta} = \hat{\mathbf{Y}} : \dot{\varepsilon}
\]  

(38)

The differential equations (37) and (38) allow a simultaneous numerical integration procedure with complete ignorance of rotational effects. The additional assumption of a uniform strain path

\[
\dot{\varepsilon} = \frac{\varepsilon(t + \Delta t)}{\Delta t}
\]  

(39)

is not in contradiction with the previous assumption regarding the incremental deformation. With relationship (39) the actual integration of (37) and (38) can be performed. The result can be expressed as

\[
\dot{\sigma}(t + \Delta t) = \sigma(t) + \hat{\mathbf{M}}_{s} : \varepsilon(t + \Delta t)
\]  

(40)

\[
\dot{\eta}(t + \Delta t) = \eta(t) + \hat{\mathbf{Y}}_{s} : \varepsilon(t + \Delta t)
\]  

(41)

An appropriate computational scheme for \( \hat{\mathbf{M}}_{s} = \hat{\mathbf{M}}_{s}(\sigma(t), \eta(t), \varepsilon(t + \Delta t)) \), to be called the rotation-neutralized averaged constitutive tensor, and for \( \hat{\mathbf{Y}}_{s} = \hat{\mathbf{Y}}_{s}(\sigma(t), \eta(t), \varepsilon(t + \Delta t)) \), the column with rotation-neutralized averaged tensors for the evolution of the history parameters, will be derived. It is noted that (40) was used in Section 2, equation (17). To account for rotational effects during the increment, application of

\[
\sigma(t + \Delta t) = R(t + \Delta t) \cdot \dot{\sigma}(t + \Delta t) \cdot R^c(t + \Delta t)
\]  

(42)

is necessary. This result was also used previously for equation (16).
The quantities $\mathbf{M}_a$ and $\mathbf{V}_a$, appearing in the expressions (40) and (41), should be calculated using a numerical procedure for the integration of the mutually coupled differential equations (37) and (38). Moreover, the iterative version of equation (40), previously formulated as (25) in Section 2, is required. This implies that an expression for the iterative rotation-neutralized constitutive tensor $\delta \mathbf{M}_i$ should also be derived. For a detailed outline of the numerical scheme applied, a concise notation for the system of equations (37) and (38) is introduced:

$$\dot{\mathbf{z}} = \mathbf{A}(\mathbf{z})\mathbf{\varepsilon}$$

(43)

The column $\mathbf{z}$ contains the components of $\mathbf{\dot{z}}$ with respect to some invariant vector base and the elements of the column $\mathbf{\eta}$. The column $\mathbf{\varepsilon}$ is composed of the components of the incremental strain tensor $\varepsilon(t + \Delta t)$. In the matrix $\mathbf{A}(\mathbf{z})$ the quantities $\delta \mathbf{M}$ and $\mathbf{\dot{V}}$ are combined. As usual, the total time range $t \leq \tau \leq t + \Delta t$ is divided into a finite number ($n$) of time steps or subincrements. A particular subincrement $i$ with $t_i \leq \tau \leq t_{i+1}$, $i = 0, 1, \ldots, n - 1$, $t_0 = t$ and $t_n = t + \Delta t$, will be considered separately. It is supposed that for $\tau = t_i$ the matrices $\mathbf{K}_i$ and $\mathbf{L}_i$ are given, defined such that the column $\mathbf{z}_i = \mathbf{z}(\tau = t_i)$ can be calculated by

$$\mathbf{z}_i = \mathbf{z}_0 + \mathbf{K}_i \mathbf{\varepsilon}$$

(44)

and that the iterative change $\delta \mathbf{z}_i$ of the column $\mathbf{z}_i$ equals

$$\delta \mathbf{z}_i = \mathbf{L}_i \delta \mathbf{\varepsilon}$$

(45)

The aim is to derive equations for $\mathbf{K}_{i+1}$ and $\mathbf{L}_{i+1}$, representing the heart of the numerical procedure. Starting from $i = 0$ (it is obvious that $\mathbf{K}_0 = \mathbf{L}_0 = 0$) with a given $\mathbf{z}_0$, all subincrements can subsequently be activated, resulting finally in $\mathbf{K}_n$ and in $\mathbf{L}_n$. With the components of these matrices, the construction of the quantities $\mathbf{4M}_a$, $\mathbf{\dot{V}}_a$ and $\mathbf{4M}_l$ can be performed easily.

For subincrement $i$ the calculations are based on the finite difference equation

$$\frac{\mathbf{z}_{i+1} - \mathbf{z}_i}{t_{i+1} - t_i} = \mathbf{A}(\mathbf{z}_i) + \frac{1}{t_{i+1} - t_i} \mathbf{\eta} \left[ \mathbf{z}_{i+1} - \mathbf{z}_i \right] \mathbf{\varepsilon}$$

(46)

with $0 \leq \zeta \leq 1$. Using Taylor expansion and solving for $\mathbf{z}_{i+1}$ yields

$$\mathbf{z}_{i+1} = \mathbf{z}_i + \left[ \frac{1}{t_{i+1} - t_i} - \zeta \mathbf{T} \left\{ \frac{\partial \mathbf{A}}{\partial \mathbf{z}} \right\}_\mathbf{z = \mathbf{z}_i} \right]^{-1} \mathbf{A}(\mathbf{z}_i) \mathbf{\varepsilon}$$

(47)

For relatively small subincrements, $\mathbf{K}_{i+1}$ is approximated by

$$\mathbf{K}_{i+1} = \mathbf{K}_i + \Delta \mathbf{K}_i (\mathbf{\varepsilon}, \mathbf{z}_i)$$

(48)

where the matrix $\Delta \mathbf{K}_i (\mathbf{\varepsilon}, \mathbf{z}_i)$ is expressed as

$$\Delta \mathbf{K}_i (\mathbf{\varepsilon}, \mathbf{z}_i) = \left[ [t_{i+1} - t_i] \mathbf{I} + \zeta [t_{i+1} - t_i] \mathbf{T} \left\{ \frac{\partial \mathbf{A}}{\partial \mathbf{z}} \right\}_\mathbf{z = \mathbf{z}_i} \right] \mathbf{A}(\mathbf{z}_i)$$

(49)

The result for $\mathbf{z}_{i+1}$, to be obtained from (44) with $\mathbf{K}_{i+1}$ for subincrement $i$, will probably violate the (active) yield criteria. To maintain consistency a correction will be performed, using a projection method. This issue will not be discussed here.

For the iterative column $\delta \mathbf{z}_{i+1}$ it can be derived that

$$\delta \mathbf{z}_{i+1} = \delta \mathbf{z}_i + \delta (\Delta \mathbf{K}_i \mathbf{\varepsilon}) = \left[ \mathbf{I} + \mathbf{\varepsilon} \mathbf{T} \left\{ \frac{\partial \Delta \mathbf{K}_i}{\partial \mathbf{z}_i} \right\}_\mathbf{z = z_i} \right] \delta \mathbf{z}_i + \left[ \Delta \mathbf{K}_i + \mathbf{\varepsilon} \mathbf{T} \left\{ \frac{\partial \Delta \mathbf{K}_i}{\partial \mathbf{\varepsilon}} \right\}_\mathbf{z = z_i} \right] \delta \mathbf{\varepsilon}$$

(50)
and for $L_{i+1}$ results with (45) the recurrence relationship

$$L_{i+1} = \left[ I + \xi^T \left[ \frac{\partial \Delta \mathbf{K}_i}{\partial \mathbf{z}_i} \right]^T \right] L_i + \Delta \mathbf{K}_i + \xi^T \left[ \frac{\partial \Delta \mathbf{K}_i}{\partial \mathbf{z}_i} \right]^T$$  \hspace{1cm} (51)

If an explicit integration scheme ($\zeta = 0$) is chosen, the relationships for $K_{i+1}$ and $L_{i+1}$ simplify to

$$K_{i+1} = K_i + \left[ t_{i+1} - t_i \right] A(z_i)$$  \hspace{1cm} (52)

$$L_{i+1} = \left[ I + \left[ t_{i+1} - t_i \right] \xi^T \left\{ \frac{\partial A}{\partial \mathbf{z}_i} \right\}_{\mathbf{z}_i = z_i} \right] L_i + \left[ t_{i+1} - t_i \right] A(z_i)$$  \hspace{1cm} (53)

The size of the subincrements can be manipulated to obtain the required accuracy. It can be arranged easily that the transition from elastic into elastoplastic material behaviour coincides with a subincremental transition. If the explicit integration scheme is applied, the number of subincrements $n$ should be larger than for an implicit scheme, in order to obtain a comparable accuracy.

The numerical simulation of powder compaction processes requires the implementation of a constitutive model in the computer software. A consideration of models in the literature makes it clear that from a physical point of view it is hard to make a well-founded choice. This justifies taking computational aspects into account. The continuity of an elliptical yield surface $^5$ offers advantages. It is supposed that the yield surface will be determined by one history parameter only. With this restriction, the permanent mass density $\rho^p$ (after local unloading) seems to be an appropriate choice for this parameter, as the compressibility of the material is considered to be of fundamental importance. Finally, an associative flow rule will be applied.

The mathematical representation for the yield criterion reads

$$f(p, q, \rho^p) = F^2 \left[ p - \frac{D + C}{2} \right]^2 + q^2 - F^2 \left[ \frac{D - C}{2} \right]^2 = 0$$  \hspace{1cm} (54)

with $p$ being the isostatic pressure, positive for compression, and with $q$ being the equivalent stress (von Mises). The cohesion is described by $C(\rho^p) \leq 0$, the densification pressure by $D(\rho^p) > 0$ and the axis ratio of the ellipse (a measure of the internal friction) by $F(\rho^p) > 0$, $F = 2q_{\text{max}}/|D - C|$. It is emphasized that the yield criterion is characterized by only three history-dependent quantities. In Figure 2 the yield surface is visualized.

Mainly following Park, $^{14}$ for $C(\rho^p)$, $D(\rho^p)$ and $F(\rho^p)$ the following empirical expressions are adopted:

$$C(\rho^p) = C_1 + \gamma D(\rho^p)$$  \hspace{1cm} (55)

$$D(\rho^p) = D_1 \left[ 1 - \frac{\rho^p}{\rho_{\text{max}}^p} \right]^\theta - 1$$  \hspace{1cm} (56)

$$F(\rho^p) = F_1 + \left[ F_2 - F_1 \right] \frac{\rho^p - \rho_{\text{ini}}^p}{\rho_{\text{max}}^p - \rho_{\text{ini}}^p}$$  \hspace{1cm} (57)

![Figure 2. Elliptical yield surface](image-url)
where \( C_1 \leq 0, \gamma \leq 0, D_1 > 0, \beta < 0, F_1 > 0 \) and \( F_2 > 0 \) represent constant material properties. \( \rho_{\text{ini}}^p \) denotes the initial material density (undeformed) and \( \rho_{\text{max}}^p \) the hypothetical maximum permanent density. Additionally, elastic behaviour is characterized by equation (32) with the isotropic constitutive tensor

\[
^4M = \lambda I + \mu [^4I + ^4I^c]
\]  

For the Lamé quantities \( \lambda = \lambda(p^p) \) and \( \mu = \mu(p^p) \) it is assumed that

\[
\lambda(p^p) = \lambda_1 + [\lambda_2 - \lambda_1] \frac{p^p - \rho_{\text{ini}}^p}{\rho_{\text{max}}^p - \rho_{\text{ini}}^p}
\]

\[
\mu(p^p) = \mu_1 + [\mu_2 - \mu_1] \frac{p^p - \rho_{\text{ini}}^p}{\rho_{\text{max}}^p - \rho_{\text{ini}}^p}
\]

with \( \lambda_1, \lambda_2, \mu_1 \) and \( \mu_2 \) having a constant positive value. The specification above contains twelve parameters to be quantified, to define completely the material behaviour.

4. NUMERICAL SIMULATION RESULTS

This section presents the results for a number of simulated compaction processes. For detailed information, not included here, reference is made to Brekelmans. The objective is to demonstrate the possibilities of the method developed. Park specified for an artificial ceramic powder the mechanical behaviour, partly based on experimental data for fine Ottawa sand. From this specification the material properties have been derived, which are used for the execution of the calculations. For the material parameters in the equations (55)–(57), (59) and (60) the values are given below.

\[
\begin{align*}
\rho_{\text{ini}}^p &= 1.86 \, \text{(g/cm}^3) \quad \rho_{\text{max}}^p = 2.70 \, \text{(g/cm}^3) \\
C_1 &= -0.04 \, \text{(GPa)} \quad \gamma = -0.05 \\
D_1 &= 0.0075 \, \text{(GPa)} \quad \beta = -1.55 \\
F_1 &= 1.4 \\
F_2 &= 0.2 \\
\lambda_1 &= 2.6 \, \text{(GPa)} \quad \lambda_2 = 15.0 \, \text{(GPa)} \\
\mu_1 &= 2.6 \, \text{(GPa)} \quad \mu_2 = 15.0 \, \text{(GPa)}
\end{align*}
\]

Firstly a compaction process in a cylindrical die is considered, visualized in Figure 3. The Coulomb friction ratio for the contact between continuum and the surroundings is taken as 0.3.
The initial height/radius ratio \( \frac{H_0}{R_0} \) is equal to 3. The punch is gradually moved down with respect to the die. The final state, with a height reduction \( \frac{H_0 - H}{H_0} \) equal to 0.25, is reached in 16 incremental steps.

Initially the total number of continuum elements was equal to 60. The elements directly under the punch were gradually reduced in dimension and removed. Figure 4 shows the distribution of the permanent density \( \rho_p \) for various stages of the deformation process. It can be observed that a considerable height reduction is necessary to obtain some material densification in the lower parts of the die. In the corner B between die bottom and die wall the density has a minimum value, and even for 25 per cent height reduction only a slight compaction is found there. The maximum density is localized in the corner C between punch and die wall, as could have been expected. Figure 5 presents the distributions of the axial stress \( \sigma_{zz} \). The occurrence of stress concentrations in the corner C is not surprising. The results obtained are globally confirmed by experiences reported in the literature.\(^7,8,13,16,18\)

The compaction of granular material in a cylindrical die can be considered as a deformation process that can be simulated with the common Lagrangian approach, as well as with the Eulerian procedure developed here. There are hardly any reasons to prefer one method to the other. As a second example a problem is analysed with material slip along non-straight parts of the continuum boundary. This example shows the advantageous capabilities of the present method. The compaction of a granular material in a cylindrical die with a concentric core is

![Diagram](image_url)

<table>
<thead>
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<th>Height Reduction</th>
<th>Density Level 1</th>
<th>Density Level 2</th>
<th>Density Level 3</th>
<th>Density Level 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.2%</td>
<td>1: 1.90 (g/cm(^3))</td>
<td>1: 1.95 (g/cm(^3))</td>
<td>1: 2.00 (g/cm(^3))</td>
<td></td>
</tr>
<tr>
<td>8.3%</td>
<td>2: 2.15 (g/cm(^3))</td>
<td>2: 2.35 (g/cm(^3))</td>
<td>2: 2.45 (g/cm(^3))</td>
<td>2: 2.60 (g/cm(^3))</td>
</tr>
<tr>
<td>16.6%</td>
<td>3: 0.05 (g/cm(^3))</td>
<td>3: 0.05 (g/cm(^3))</td>
<td>3: 0.05 (g/cm(^3))</td>
<td>3: 0.05 (g/cm(^3))</td>
</tr>
<tr>
<td>25.0%</td>
<td>4: 0.05 (g/cm(^3))</td>
<td>4: 0.05 (g/cm(^3))</td>
<td>4: 0.05 (g/cm(^3))</td>
<td>4: 0.05 (g/cm(^3))</td>
</tr>
</tbody>
</table>

Figure 4. Distributions of the permanent density
DIE COMPACTION PROCESSES

height reduction: 4.2%
level 1: -0.10 (GPa)
level 7: -0.03 (GPa)
step: 0.01 (GPa)

level 1: -0.18 (GPa)
level 8: -0.04 (GPa)
step: 0.02 (GPa)

level 1: -0.36 (GPa)
level 8: -0.08 (GPa)
step: 0.04 (GPa)

level 1: -1.30 (GPa)
level 13: -0.10 (GPa)
step: 0.10 (GPa)

Figure 5. Distributions of the axial stress

Figure 6. Compaction in a cylindrical die with concentric core
analysed. In Figure 6 the initial configuration is shown, while the mesh with continuum elements for increment 1 is also visualized.

Coulomb's friction ratio was taken as 0.3. The punch was incrementally moved down in 6 steps equal to 0.11. The continuum was divided into 67 elements for increment 1, reduced to 62 elements for increment 6. For increment 6 the results are presented in Figure 7.

For all increments computed, stick was found at point B. Just below point B the density gradient proves to be relatively high. It can be observed that in that area positive axial stresses occur, which is certainly not surprising. Directly under the punch similar phenomena are found, as for the previous example. Above the top of the core near point B an area with increased
compaction results. Experimental research into compaction in a similarly shaped die as considered here, reported by Morimoto et al.,\textsuperscript{11} broadly confirms the results derived with the present method.

It is noted that the element mesh used for this configuration is definitely not quite refined enough to produce reliable results in the neighbourhood of point B. The rough discretization is unsuitable to represent the distributions of the relevant quantities in an adequate manner. It is obvious that with a finer element mesh an improved accuracy can be reached. Within the scope of the present research there was no reason to really execute such a computation.

The Eulerian approach allows a simple examination of the influence of (small) modifications in the problem description. Smoothening of the corner at point B is obtained by reallocation of the node in point B only. In this way the radius of curvature simulated approximately equals 0.25L. With an identical incremental procedure as applied before, the calculation is repeated. The results are displayed in Figure 8.

For the new situation slip is clearly observed at the boundary near B. For the node in B the incremental slip equals 0.0071 for increment 1 and increases gradually up to 0.011 for increment 6. A comparison of Figure 7 with Figure 8 shows some minor differences. The adaptation of the geometry apparently only affects locally the process.

5. CONCLUSIONS

It has been shown that the Eulerian approach is suitable for analysing die compaction processes. The finite element configuration is not influenced by the material displacements. Consequently, mesh rezoning is not necessary to properly describe material slip along non-straight die edges. In the procedure presented in Section 2, remeshing is prescribed in advance by the specified volume reduction and therefore an automatic incrementation can be executed easily. Besides, to investigate the effect of, for instance, changes in the material properties, the original incremental element meshes suffice.

For the solution of the resulting set of non-linear equations a Newton-Raphson scheme has been applied. It has been shown how consistent iterative relationships between variations of strain and stress can be derived simultaneously with the numerical integration of the constitutive equations. The calculation method proposed in Section 3 is generally applicable in the field of elastoplasticity.

REFERENCES


