Compaction of Aggregated Ceramic Powders, Discrete Element and Finite Element Simulations

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Abstract

In contrast with the Finite Element Method, the Discrete Element Method (DEM) takes explicitly into account the particulate nature of powders. DEM exhibits some drawbacks and many advantages. Simulations can be computationally expensive and they are only able to represent a volume element. However, these simulations have the great advantage of providing a wealth of information at the microstructural level. Here we demonstrate that the method is well suited for modelling, in coordination with FEM, the compaction of ceramic UO_2 particles that have been aggregated. Aggregates of individual ceramic crystallites that are strongly bonded together are represented by porous spheres.

Keywords : Powder compaction, Discrete element simulation, Finite element simulation, Uranium dioxide

1. Introduction

Cylindrical nuclear fuel pellets are generally obtained after a sintering stage from green compacts formed by die-compaction. Gradients of density in the green compact are originally induced during the stage of compaction and may induce a heterogeneous shrinkage during sintering, which influences the final shape of the pellets. For example, in the double action compaction, the pellet is thinner in the median plan. This phenomenon is generally defined as hour-glassing. Regrinding is thus necessary to ensure required dimensions. In this context, analytical model and numerical simulations are used to predict sintered and green part dimensions or crack initiation [1-6].

The continuum mechanics approach such as the Finite element method (FEM) allows modelling of the entire part, but the granular characteristics of the powder cannot be taken into account. In contrast, the Discrete Element Method (DEM), takes the granular behaviour of the powder in full account [3-6]. However, CPU time requirements do not allow the whole part (containing several millions of particles) to be considered since each particle and each contact between particles is modelled separately in DEM. Periodic boundary conditions may be used instead to model a Representative Volume Element, leading to a wealth of information at the particle length scale [7].

This work explores the possible use of DEM to generate constitutive equations to feed a FEM code that can in turn model the whole part. Typically DEM simulations are able to generate yield and fracture surfaces that are otherwise extremely difficult to obtain experimentally [5,6]. Previous experimental data on UO_2 powder are used in combination with FEM, to fit the contact law material parameters.

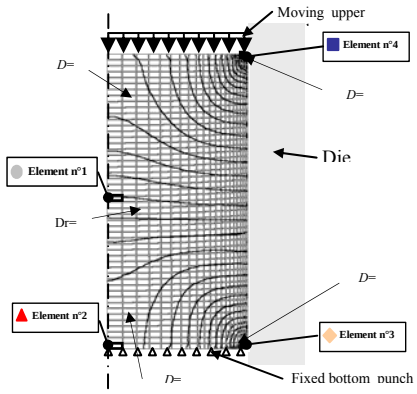

Fig. 1. Mesh boundary conditions and relative density contour at maximum loading (600 MPa).

2. Finite element simulations

The FEM code CASTEM was used to simulate the close die compaction of uranium powder as a 2D axi-symmetric problem (Fig 1). Single acting die compaction is modelled and constant friction is assumed with the die.

A simplified Cam-Clay model is used to model the powder behavior. The PreCAD® numerical simulation tool was used to calibrate the Cam-Clay model. Calibration was carried out by using experimental data

determined from die compaction of a UO_2 powder obtained through the ammonium diuranate process.
Fig. 1 shows the relative density contours of the green compact computed by FEM simulations for a 600 MPa applied stress on the upper punch. The largest local densities were located at the upper rim, whereas the lowest densities were located at the bottom rim. Density gradients were less important in the core of the pellet than in the circumference zone. These results agree qualitatively with the experimentally determined density distribution in a UO_2 cylindrical compact [8,9]. The location of selected elements is given in Fig 1. The macroscopic behavior of the pellet was studied by using the average stress calculated by Jansen's model on the median plane [10]:

$$\bar{\sigma} = \sqrt{\sigma_{sup} \cdot \sigma_{inf}} \qquad (1)$$

where σ_{sup} is the upper punch stress and σ_{inf} is the transmitted stress on the bottom punch.
Fig. 2 illustrates the comparison between the local and the macroscopic behavior of the powder. The average axial stress ($\bar{\sigma}_z$) curve is plotted as a function of the average macroscopic relative density whereas the local axial stresses (σ_z^i) are plotted versus the local density for each element. The local and average results are located approximately on the same curve. Thus, eqn (1) can be used in order to fit the DEM compaction curve. Fig. 2 demonstrates that if σ_{sup} and σ_{inf} are known from experimental data, the simple use of eqn (1) gives access to the local constitutive behaviour of the powder. Also, FEM calculations have shown that the fluidity index (ratio between the transverse and axial stresses) is approximately homogeneous in the bulk of the compact.

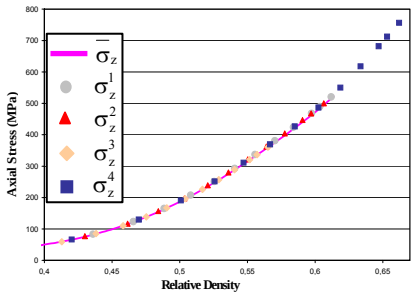

Fig. 2. Average axial stress ($\bar{\sigma}_z$) versus average relative density and local axial stress versus local relative density for each selected element (σ_z^i) shown in fig. 1.

3. Discrete Element simulations

The DEM code dp3D [3,5], is used to model a REV of the ceramic compact. UO_2 powder is typically made of aggregates (~ 10 μm size) that contain a number of crystallites (~ 100 nm particule size) strongly bonded together. Here, each aggregate is represented by a porous sphere with relative density $D_{agr} = 0.64$. Thus, the relative density of the DEM sample is simply given by the product $D_{agr}D_{packing}$ where $D_{packing}$ is the relative density of the sphere packing. The normal contact force between two aggregates is given by a hardening plasticity contact law:

$$N = K \cdot R^{*(1-\frac{1}{2 \cdot m})} \cdot h^{(1+\frac{1}{2 \cdot m})} \qquad (2)$$

where, m is the hardening coefficient, K is a constant, R^* is the harmonic average radius and h is the indentation between the two spheres.
Fig. 3 shows the compaction curves from experimental and DEM results. The experimental average stress is calculated with eqn (1). The compaction curve is well fitted by the DEM simulation above 100 MPa. This compaction stage corresponds to the rearrangement and/or fracture of aggregates. Before this stage, rearrangement and fracture of agglomerates of aggregates (size of 100 - 300 μm) is the dominant densification mechanism.

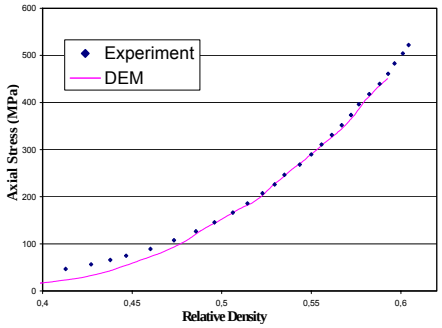

Fig. 3. Compaction curves: Experimental data and DEM results

4. References

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