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Numerical modeling of cold powder compaction using multi particle and continuum media approaches

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Numerical analysis of powder compaction process requires multi-particle modeling approach as continuum models fail to simulate the nature of process (e.g. interparticle, and particle–die interactions), accurately. This study aimed for analyzing powder compaction process utilizing 3-D finite element modeling approach along with different material models including modified Cam-Clay, Mohr–Coulomb, Shima–Oyane and von-Mises. The finite element analyses were carried out by implementing multi-particle finite element method. Moreover, continuum modeling was also performed for comparison purposes. In both cases, the compaction of spherical copper particles was analyzed at room temperature conditions. The obtained FEA results were compared in terms of equivalent stress and strain, and deformed shape. Results showed that the FE models in which von-Mises and modified Cam-clay material models were used yielded results of similar magnitude while those of Shima–Oyane and Mohr–Coulomb material models resulted in equivalent stress and strain values are in close proximity. Effect of coefficient of friction on the results was also investigated by implementing three distinct coefficients of friction (μ = 0.1, 0.25, 0.4). It was noted that increasing friction resulted in elevated level of deformation for the particles and harsher particle–particle, and particle–die contact interactions.

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1. Introduction

Powder metallurgy (PM) is a general term for manufacturing nearnet or net shape manufacturing parts from metal and alloy powder mixtures. It offers several advantages including ability to produce parts made of wide spectrum of materials, control over the shape, size and porosity of the part, tailoring physical and mechanical properties as desired, suitability for mass-production, elimination of post-processing (deburring, e.g.) in most cases, cost effectiveness over casting, forging, and machining etc. PM has found applications in several industries; including automotive, aerospace, consumer goods, computers, defense, medical, power tools, etc. The most common parts produced through powder metallurgy are filters, bearings, high-strength tools, forming die, and inserts, as well as pharmaceutical tablets, detergents, etc. Market size estimations, on the other hand, for powder metallurgy products grow up every year. It is reported that the production of metal powders that are used by various industrial consumers valued more than 4 billion USD per year solely in North America [\[1\]](#page--1-0).

Cold powder compaction process, specifically, produces unsintered parts called "green body" in room temperature. The flow behavior in cold powder compaction has been investigated by many authors in last decades. Continuum media approach, Discrete Element Method (DEM), and Multi Particle Finite Element Method (MPFEM) are the main modeling approaches in powder compaction simulations.

In the continuum media approach, particles were considered as continuous isotropic medium disregarding the inter-particle contact interactions. Residual stresses in metal powder compaction process can be analyzed by continuum approach. It introduces visco-plastic solutions in soil mechanics for non-cohesive granular volumes [\[2\]](#page--1-0). Tablet compaction of pharmaceuticals [\[3\],](#page--1-0) and large deformations in compaction process were successfully handled via continuum approach as reported in literature [\[4,5\].](#page--1-0)

Discrete element method (DEM), also referred as to "distinct element method", on the other hand, was developed by Cundall in 1971 for rock and soil mechanics problems, where motion of particles were analyzed through Newton's second law of motion by taking contact interactions between particles into account [\[6,7\],](#page--1-0) and handling contact forces as functions of the particle overlap [\[8\].](#page--1-0) The method was used to analyze problems in various fields including granular flow patterns and stress fields of solids stored in silos [\[9\]](#page--1-0), granular milling, conveyor transfer of granular materials, and their storage etc. [\[8\]](#page--1-0). In addition, cylindrical tablet compaction process was analyzed through commercial finite element analysis package, and that DEM was noted as an efficient method to simulate these types of processes [\[10\]](#page--1-0). In early DEM modeling, particles were modeled as rigid, however; after algorithmic modifications, DEM became available for elasto-plastic analysis, as well. As opposed to most powder material models, high density compaction process can also be simulated by this approach. For example, Jerier

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et al. described a high density model for powder materials using the open source YADE software with Voronoi cells [\[11\].](#page--1-0) DEM assumes that the granular materials/particles were circles in 2D or spheres in 3D and can overlap or detach [\[12\].](#page--1-0) The main drawbacks of DEM calculations were a) limitation of number of particles in simulation of real particles due to high performance computational platform needs and/or time concerns [\[9\];](#page--1-0) b) use of simplified contact interactions [\[13,14\]](#page--1-0), inability to obtain normal and shear stress with rigid DEM particles [\[15\].](#page--1-0) Therefore some researchers integrated DEM with finite element method (FEM) by taking the advantage of both continuous and discrete approaches [\[16](#page--1-0)–18]. Harthong et al. used discrete finite element simulations to study relations between loading history and yielding surfaces aiming to define strain hardening of metal powders [\[19\].](#page--1-0)

Improved accuracy in particle simulation along with incorporation of detailed contact laws, defining arbitrary material properties for granular particles was realized through finite element modeling. It was first implemented by Ransing et al. and has been developed since then [\[20\].](#page--1-0) This approach is also called as multi-particle finite element method (MPFEM) [\[13\]](#page--1-0). Procopio and Zavaliangos used MPFEM approach to explore the densification of granular media under multi-axial compaction effect [\[14\].](#page--1-0) It was concluded that MPFEM provided necessary degrees of freedom that allows for local non-uniform contact deformation which was not available in DEM. Zhang studied local non-uniform contact deformation and nonuniformity stress chains of compaction of different size particles in soft and hard composite mixtures using MPFEM [\[21\].](#page--1-0) MPFEM introduce more accurate result in the simulation of models which have nonlinear particle interactions in discontinuous environments. In MPFEM, different material properties can be assigned to each particle and element coarsening or other properties of the particles may differ from each other. MPFEM define all particles as a solid continuum elastic–plastic bodies which can initially be defined either gluing or touching each other. It was used to simulate effect of punch displacement on cold compaction of Al particles in 2D by Lee et al. [\[22\].](#page--1-0) Gustafsson et al. showed in their research that MPFEM simulation for compaction of iron ore pellets agreed well with experimental results [\[8\].](#page--1-0)

Although the above mentioned studies provide valuable information on cold powder compaction process, they only focused on one material model and did not take the interactions between the individual spherical particles into account. Therefore, this study aimed for revealing the effects of different material models namely von-Mises, modified Cam-Clay Shima–Oyane, and Mohr–Coulomb, and contact conditions on interactions of individual spherical copper particles and die wall in a cold compaction process. In order to achieve this goal, each particle was modeled as individual deformable body with 3D tetrahedral elements through MPFEM approach. In addition to MPFEM approach, continuum modeling approach was also performed for comparison purposes. Next sections introduce the experimental work performed earlier [\[23\]](#page--1-0) and the current numerical study based on this experimental work.

2. Description of physical process and MPFEM model

Fig. 1 shows the die model geometry and powder compact product which is taken as reference for the current study [\[23\].](#page--1-0) Such modulated surfaces were noted as capable of providing increased heat transfer rates up to %300.

Particles of 200 micron in diameters were first modeled as solid spheres in Solidworks (Solidworks Corp., Waltham, MA, USA). Those then were filled into single die cavity with free-falling effect in order to achieve random distribution of particles in die cavity. Solid spheres were then converted into 74 elastic–plastic isotropic discrete deformable bodies (particles), yielding a total number of 60,076 3-D tetrahedral elements and 15,255 nodes shown in [Fig. 2](#page--1-0). Model preparation was handled in MSC Patran (MSC Software Corp., Santa Ana, CA, USA) upon mesh convergence testing. An important factor in convergence ratio is setting the element type properly. Tetrahedral element was chosen instead of hexahedral or other possible element types to lower the computational time. Optimum numbers of tetrahedral elements were determined upon MPFEM analyses with different number of elements. [Fig. 3](#page--1-0) shows variation of maximum equivalent (von-Mises) stress values with respect to number of elements used in FE models.

The 3-D FE model with 60,076 3-D tetrahedral elements was then imported to commercial FEA package MSC Marc Mentat, and material properties, contact parameters, convergence parameters, and friction model were defined prior to analyses. In terms of numerical preferences, the residual or displacement testing option was used as convergence testing criteria. Implicit solution technique in combination with full Newton–Raphson iterative procedure was preferred as numerical solution algorithm. Coulomb bilinear (displacement) friction model with coefficient of friction value of $\mu = 0.1$ was defined for all contacting interfaces. Moreover, the effect of different friction coefficients (μ = 0.1, 0.25 and 0.4) on results was investigated in [Section 4.3.](#page--1-0)

In addition to multi particle FEA, continuum FEA of powder compaction was also studied for comparison purposes. [Fig. 4](#page--1-0) shows the continuum FE model consisting of one deformable body in contact with die involving 46,644 tetrahedral elements. Incremental remeshing procedure was defined for an improved convergence. Coulomb bilinear displacement type of friction model was implemented in die wall–particle interface. FE analyses were performed in commercially available MSC Marc software (v. 2012.1.0) using a PC equipped with an Intel Core i7 2.20 GHz processor, and 8 GB RAM.

3. Material models

Material model selection is one of the critical issues in finite element modeling to represent the deformation behavior of particles, accurately. In literature, there is no consensus on a specific material model, and one

Fig. 1. a) Dimensions for compaction die (in mm), and b) SEM micrograph; c) final shape of the produced part [\[23\]](#page--1-0).

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