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Real-Time Design of Improved Powder Pressing Dies Using Finite Element Method Modeling

K. G. Ewsuk, J. G. Arguello, D. H. Zeuch, and A. F. Fossum

Prepared by
Sandia National Laboratories
Albuquerque, New Mexico 87185 and Livermore, California 94550

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Dies Using Finite Element Method Modeling**

K. G. Ewsuk
Ceramic Materials Department

J. G. Argüello
Solid Mechanics Engineering Department

D. H. Zeuch
Geomechanics Department

A. F. Fossum
Materials Mechanics Department

Sandia National Laboratories
P. O. Box 5800
Albuquerque, NM 87185-1349

Abstract

A predictive model for powder compaction has been developed that incorporates unprecedented flexibility to design powder press tooling and reliable powder pressing processes. Sandia's finite element (FE) toolkit comprises the heart of the modeling software, and a unique concept was developed to design a variable dimension and parameter template to easily build/design dies/components on a computer. The result is user-friendly software to simulate powder compaction that can run on a desktop or laptop personal computer by a non-expert with minimal training. The software has been tested and validated by direct comparison to experimentally measured density gradients in green ceramic powder compacts. The software has been used successfully to enhance our fundamental understanding of ceramic powder pressing, and has provided guidance to achieve better process reproducibility, reliability, and control. This technology will contribute significantly to press powder manufacturing by: 1) reducing manufacturing costs, cycle time, and waste; 2) enabling more cost effective manufacturing of specialty components and small lot sizes; 3) reducing tooling and component design, development, and prototype time; and 4) maximizing design and manufacturing flexibility/agility.

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Introduction

Dry powder pressing is the most common method used to form components in the ceramic manufacturing industry [1-3]. Ideally, the object of dry pressing is to quickly and reproducibly form a homogeneously dense powder compact to near-net-shape. However, defects in the form of density gradients are common in pressed powder compacts. While it is not practical to completely eliminate density gradients from a pressed powder compact, it is imperative to minimize such gradients to have an economical forming process that produces reliable components.

In general, macroscopic density gradients are undesirable because they contribute to differential sintering and warping (i.e., shape distortion) that can necessitate costly diamond grinding to produce the desired final size and shape part [4]. Additionally, macroscopic density gradients can produce defects that limit the performance and reliability of the finished part. Typically, macroscopic density gradients are produced by non-uniform die filling and/or forming pressure gradients present during powder compaction [1,4-6]. To avoid introducing density gradients, precautions must be taken to optimize the stress transmission and stress uniformity throughout the powder compact during pressing. Experienced press operators generally accomplish this by understanding and controlling parameters such as die fill density, die wall friction, and pressed compact expansion on ejection. However, this is very much an art.

Generally, a combination of practical experience and trial and error are used to design ceramic components and the dry pressing processes used in ceramic component design and manufacturing. This involves designing a part from practical experience, machining the tooling (i.e., punch and die assembly) to make the part, pressing a prototype to test the design, and redesigning and retooling. Because there can be numerous iterations before going into production, this process is inefficient, costly, unreliable, and can seriously limit component designs and pressing processes.

Modern technology that allows one to predict compaction response can now serve to guide die design and ceramic powder pressing. Models for powder compaction have been successfully developed and used to predict the density gradients and shape distortions in both ceramic and metal powder compacts[7-12]. Furthermore, using a combination of die design and green machining before firing, compaction modeling has been used to design and manufacture specialty ceramic components that can be fired to near-net shape[11]. These models utilize finite element (FE) method numerical modeling technology to predict localized stresses and strains within a powder bed continuum to simulate powder compaction. The exact relationship between stress and strain, and ultimately the density in the compact are determined by the constitutive behavior of the specific material of interest [7,12]. The accuracy of the FE model predictions depends on

the validity of the constitutive materials model as well as the accuracy of the powder properties that feed into the FE analysis. Realistic predictions of the spatial density variations within a ceramic powder compact have been made using a cap-plasticity model to describe the constitutive behavior of the ceramic powder during compaction [12].

FE modeling is a powerful tool that is becoming increasingly used in materials design and engineering. However, FE models typically require an expensive computer workstation, and specialized expertise in computing and mechanics to correctly set up and run analyses, and interpret the results.

The objective of this work was to develop new technology to make die design and powder pressing a science that can be more readily understood and controlled. The intent was to integrate materials and process engineering expertise with FE computer modeling expertise to develop software for die design and powder compaction. To circumvent the need for specialized capabilities and expertise in computing and/or mechanics, there was a specific interest in developing a user-friendly compaction software package that an informed layman could run on a personal computer.

Powder Compaction Modeling Software

FE modeling of ceramic powder compaction was accomplished using a cap-plasticity constitutive model [12]. A generalized version of the Sandler-Rubin [13] cap-plasticity constitutive model was selected because it captures the mechanical behavior of a granulated ceramic powder during compaction reasonably well. This constitutive model is comprised of a stationary shear failure surface and a strain-hardening cap that define the bounds of the elastic regime for the compaction of a powder in response to both hydrostatic compression and shear (see Figure 2 in Appendix A).

The cap-plasticity constitutive model was implemented within the JAS3D FE computer code, which is a three-dimensional (3D) numerical simulation computer program for nonlinear, inelastic, large-scale deformation problems [14,15]. A pre-processing tool is used to construct the finite element mesh required as input into JAS3D, and a post-processing tool is used to visualize the output of the FE analysis. In combination, the resulting FE toolkit can be used to predict forming stresses, density gradients, and material flow to evaluate the effects of pressing conditions, compaction ratio, die design, and die wall friction coefficient in even the most complicated 3D geometry compacts imaginable (**Figure 1**). However, effective use of the software at this level requires significant FE meshing and modeling experience, insight into the mechanics of powder compaction, and considerable experience with the cap-plasticity constitutive model.

To produce a more user-friendly software package, a higher-level of specialized software was integrated with the general FE toolkit (see Figure 5 in Appendix A). This specialized software, called UNIPACK, allows a layman with minimal training to model powder compaction for a specific subclass of variable-geometry, axisymmetric compacts. UNIPACK is a top-level driver that queries the user for information to run the FE simulation, builds the input files and the FE mesh, automatically runs the compaction analysis, and automatically displays the density gradient results.

The flexibility to model simple and complex geometry components was achieved by developing the UNIPACK code, which employed a new concept that allows the design of a variable dimension and parameter template to build/design dies on a computer in real time. This was accomplished by treating a more complex geometry component as an assembly of simpler geometry parts (see Figure 4 in Appendix A). The simple geometry units within a stack can be solid or hollow, and can have variable inner and outer diameters, and heights. Different size and shape component geometries (e.g., counter-bores and bushings) are produced by axially linking individual units of different geometry. For example, the bushing geometry illustrated in **Figure 2** was constructed from two concentric cylinders stacked axially and interconnected with smaller radii joints (see Figure 6 in Appendix A).

In addition to providing a simple and easy method to vary component/tooling geometry, UNIPACK also provides the capability to realistically vary the properties of the powder press tooling material (e.g., die wall friction coefficient). Additionally, UNIPACK allows the user to systematically vary the pressing process by varying the displacement of the top and/or bottom pressing punch. For example, **Figure 3** shows the results of a compaction simulation in which a tube was pressed uniaxially by single-action pressing from the top down, and uniaxially by dual-action pressing from the top down and the bottom up simultaneously.

UNIPACK also allows the user to vary the properties of the powders being pressed. Three different ceramic powder systems were completely characterized, and resultant data was reduced and incorporated into the UNIPACK code to use as input for ceramic powder compaction simulations.

Finally, within the code itself, the logic has been developed to design more complex geometry, axisymmetric dies, and base templates have been designed to model isostatic compaction of complex geometry parts.

The compaction modeling software was originally developed and run on a Sun workstation using the Unix operating system. It was subsequently ported over to a PC platform where it runs using the Linux operating system. Three dimensional compaction

simulations with up to 50,000 elements can be run on the PC platform. A relatively small simulation with 30,000 elements takes about 30 minutes of CPU time to run using a 450 MHz Intel Pentium III chip.

The specialized compaction software allows users with little or no FE expertise to benefit from the tremendous power and insight that FE analysis can bring to the design cycle. Furthermore, as the user develops expertise in modeling the powder compaction process, the more general underlying software is available to model more complicated geometries and processes.

Characterization of Powder Properties for Modeling

To support the new simulation tool developed for ceramic powder compaction, soil mechanics techniques were refined and applied to characterize granulated ceramic powders and obtain the input parameters required for the simulations. Ceramic powders and powder compacts were characterized using hydrostatic and triaxial compression tests [16]. These tests provided the data necessary to define the shear failure and hardening cap surfaces that make up the cap-plasticity constitutive model (see Figure 2 in Appendix A). Additionally, these same tests allowed us to measure or calculate the remaining bulk properties (i.e., powder compact bulk modulus, shear modulus, and Poisson's ratio) required to model ceramic powder compaction [12,16].

Initially a spray-dried 94 wt.% alumina powder containing 3 wt.% of a cellulose binder was characterized, and techniques were developed to reduce the data generated to obtain the material parameters required as input for the FE compaction model simulations. Subsequently, two additional ceramic powders with different degrees of pressability were characterized, and the properties of all three different powders were incorporated into the UNIPACK interface.

Powder Compaction Model Validation

Testing and validation of the FE compaction software package was accomplished through a combination of compaction simulations and by comparison of the predicted results to the characteristics of actual components pressed from granulated ceramic powders.

To initially verify that the cap-plasticity constitutive model had been implemented correctly within the FE model, one of the triaxial compression tests completed to characterize the properties of the 94 wt.% alumina powder was simulated. The entire

loading history for the test, completed at a confining pressure of 68.9 MPa, was accurately simulated (see Figure 3 in Appendix A).

Having established basic confidence in the model, more complex simulations were performed. Using the measured data for the 94 wt.% alumina powder in combination with a realistic estimate of the die wall friction coefficient (i.e., 0.20 - 0.40), compaction simulations were completed on several different powder compact geometries. The validity of the compaction model was assessed qualitatively by comparing general trends from the model predictions to those determined by direct observation. To complete a quantitative assessment, the model-predicted density gradients were compared to the measured density gradients in an actual powder compact after pressing. The most quantitative density data for a powder compact was obtained using ultrasound velocity measurements with density standards.

A cylindrical compact geometry was selected to complete a quantitative assessment of density gradients in comparison to compaction model predictions. A cylindrical sample of 94wt.% alumina was formed by single-action pressing at 68.9 MPa (10,000 psi) using a Carver uniaxial hand press. The part was pressed from the top down, and the bottom plunger remained stationary. Ultrasound velocity measurements required a bisque-fired sample with flat and parallel surfaces. The compact was bisque-fired by heating at 10°C/min to 1300°C (2372°F) [17]. A short hold time of 10 minutes was used to ensure little or no change in the compact density during firing. Longitudinal slices were cut from the compacts and milled flat and parallel to the desired thickness. Density standards in the range of 50% to 56% were also fabricated by pressing low aspect ratio alumina compacts at pressures ranging from 34.5 to 137.8 MPa. (5,000 to 20,000 psi, respectively). Ultrasound velocity measurements were made on the samples using the pulse-echo mode at 5 MHz with a 5 mm transducer [17].

The compaction of the 94wt.% alumina cylinder was simulated using a compaction ratio of 1.9 to approximate the 68.9 MPa forming pressure. Single-action pressing from the top down was modeled using the properties of the 94wt.% alumina powder and a die wall friction coefficient of 0.25.

In both the experimental results and the compaction model predictions shown in **Figure 4**, the outer diameter of the powder compact adjacent the pressing punch showed the highest density, and the outer diameter adjacent the stationary punch showed the lowest density. And in both cases, density decreases axially with distance from the pressing punch. The compaction model predicted a relative density of 0.56-0.57 at the outer top of the compact, and a relative density of 0.50-0.51 at the outer bottom. These predictions compare quite well with the respective measured values of 0.56 and 0.50.

While the model does a good job of predicting spatial density variations in the compact, it is not perfect. The predicted spatial distribution of relative density is somewhat different in the radial direction near the top and near the bottom of the cylinder. These differences are attributed to some of the assumptions and simplifications used in the model. In particular, in the simulation, material was free to move radially and axially relative to the punch faces, as no friction was considered at the punch surface. Realistically, die wall friction at the punch faces can be expected to affect powder compaction and the resultant density gradients after compaction. A second assumption in the model is that powder packing in the die was completely uniform at the start of compaction. Previous work suggests that this is highly unlikely in a real part [5,6]. Finally, the coefficient of friction between the die-wall and the powder may be different from the assumed value, or the frictional interaction may not be simple Coulomb friction. Improvements in the ability of the FE compaction modeling software to quantitatively predict spatial density variations may be realized by addressing these issues.

Compaction Model Applications

A model for ceramic powder compaction has been developed, tested, and experimentally validated. This model represents a powerful and promising new tool that can be applied to better understand and control die/component design, and the powder pressing process.

The compaction modeling technology developed can be used to troubleshoot existing processing problems to improve yields, reduce waste, and develop more efficient manufacturing processes for problem parts. Some improvements can be realized with minor modifications in die design and/or the pressing process. The compaction model also can be used to improve tool and die design by identifying and addressing design problems in the initial stages of a project. The compaction software also can be used to identify potential problems and refine die designs prior to production. Tooling can then be designed with customer input, significantly reducing design and prototyping costs. Furthermore, it is reasonable to anticipate that the compaction software can help ceramic component manufacturers expand the current design limits, which could lead to new products for new markets. A significant economic impact could be realized by designing parts that fire to net-shape without the need for green machining and/or hard grinding (i.e., diamond grinding) after sintering.

In addition to simulating powder pressing, the compaction model also provides a means to relate powder properties and characteristics to pressing behavior. Creating a good pressing powder is the first step towards a robust manufacturing process and the production of reliable components. The compaction model can provide a systematic means of assessing and understanding cause and effect between powder characteristics

and powder compaction to optimize press powder manufacturing. Similarly, the compaction model may also be able to provide valuable information about ceramic powders and their limitations in pressing. Different powders have different compaction responses, and not all powders can be pressed to all geometries. More complex geometry powder compacts can be formed from more pressable powders, but there are limitations for harder-to-press powders. Compaction simulations can be used to assess and rank-order powders in terms of pressability, and to establish use limits for certain powders. Eventually, in combination with readily measurable powder characteristics, it may even be possible to employ FE compaction modeling with basic powder data to guide the design and development of more pressable powders.

Summary

Overall, compaction modeling can provide a more comprehensive understanding of the compaction process, identify critical process parameters, and define the design and process control necessary for net-shape pressing. The application of compaction modeling to develop more robust pressing operations, design better press tooling, and to develop better pressing powders will be a major step towards developing more reliable, efficient, and cost effective processes for manufacturing ceramic powder compacts.

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Figures

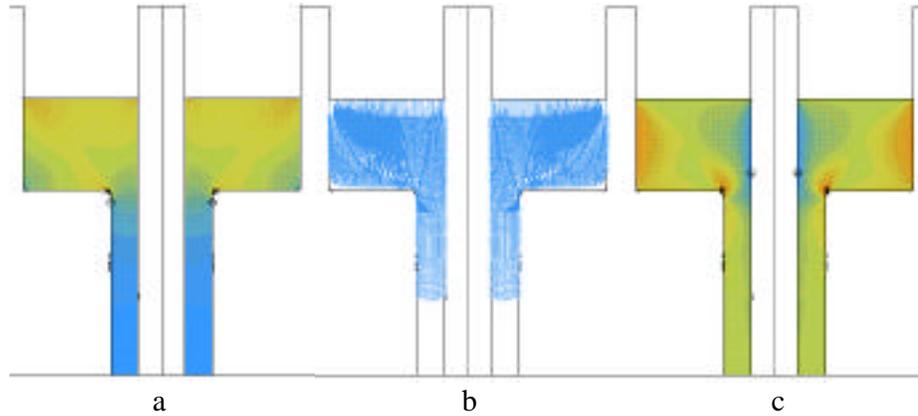


Figure 1. An FE model simulation of powder compaction in bushing, pressed uniaxially from the top down, showing a two-dimensional cross-section of the predicted: a) density gradients; b) material displacement; and c) shear stresses. Density and shear stress change with color, with blue < green < yellow < orange < red. The maximum density and shear stress are identified by an *. The minimum density and shear stress are identified by an . Note the poor densification and material flow into the bottom flange, and the high shear stress gradient at the transition radius from the head to the bottom flange. The simulations were completed using the material properties of a diatomaceous earth and a die wall friction coefficient of 0.4.

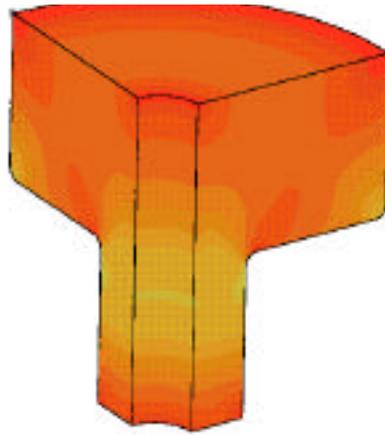


Figure 2. The density gradients predicted by the FE compaction model in a quarter section of a 94 wt.% alumina bushing pressed uniaxially by dual-action pressing. The maximum density is identified by an * in the figure. Density uniformity was optimized by controlling the punch displacements relative to original height of the head and bottom flange at 2 and 1.69, respectively (i.e., where a value of 2 signifies the pressed height of the head was 1/2 that of the original fill height).

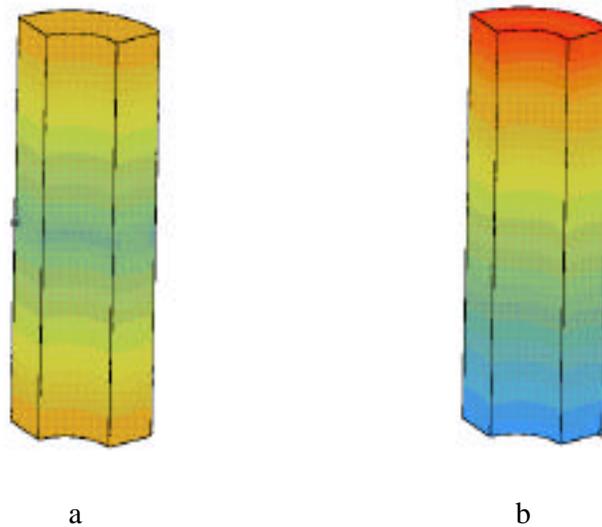


Figure 3. The density gradients predicted by the FE compaction model in a quarter section of a 94 wt.% alumina tube. The 25.4 mm long tubes were compacted uniaxially at 103.4 MPa by: a) dual-action pressing; and b) single-action pressing from the top. Density changes with color, with blue < green < yellow < orange < red (e.g., from bottom to top in tube b). Smaller gradients in density are achieved by dual-action pressing, which moves the low density region from the bottom of tube b to the middle of tube a. The maximum density is identified by an * in the figure. The minimum density is identified by an .

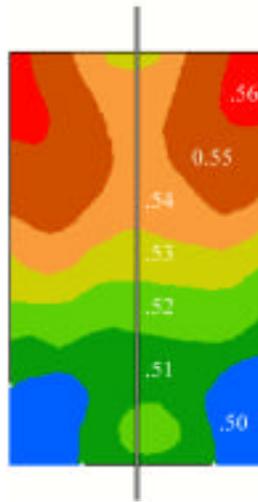


Figure 4. The density gradients through the cross section of a cylindrical powder compact of 94 wt.% alumina after uniaxial pressing at 69 MPa measured by ultrasound velocity measurements completed on a bisque-fired part.

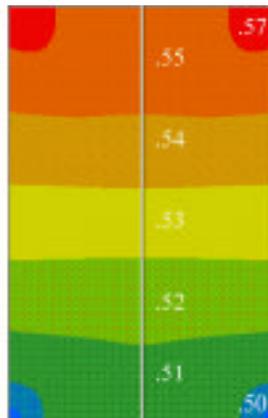


Figure 5. The density gradients through the cross section of a cylindrical powder compact of 94 wt.% alumina after uniaxial pressing at 69 MPa predicted using the FE compaction model assuming a die wall friction coefficient of 0.25. The model simulations, which show good agreement with the measured density gradients, did not consider the friction effects on the pressing punches or the initial density variability from die filling in the analysis.

Appendix A – J. G. Argüello, A. Fossum, D. Zeuch, and K. Ewsuk, “Continuum-Based FEM Modeling of Alumina Powder Compaction” to be published in *KONA Powder and Particle* [19], 2001.

CONTINUUM-BASED FEM MODELING OF ALUMINA POWDER COMPACTION

J. Guadalupe Argüello, A. F. Fossum, D. H. Zeuch and K. G. Ewsuk

Sandia National Laboratories

P. O. Box 5800 – MS 0847

Albuquerque, New Mexico, USA 87185-0847

ABSTRACT

Software has been developed and extended to allow finite element (FE) modeling of ceramic powder compaction using a cap-plasticity constitutive model. The underlying, general-purpose FE software can be used to model even the most complex three-dimensional (3D) geometries envisioned. Additionally, specialized software has been developed within this framework to address a general subclass of axisymmetric compacts that are common in industry. The expertise required to build the input deck, run the FE code, and post-process the results for this subclass of compacts is embedded within the specialized software. The user simply responds to a series of prompts, evaluates the quality of the FE mesh that is generated, and analyzes the graphical results that are produced. The specialized software allows users with little or no FE expertise to benefit from the tremendous power and insight that FE analysis can bring to the design cycle. The more general underlying software provides complete flexibility to model more complicated geometries and processes of interest to ceramic component manufacturers but requires significantly more user interaction and expertise.

INTRODUCTION

Conventional ceramic component manufacturing often involves processing and fabrication with raw materials in powder form. Granulated powder is formed into a “green” body of the desired size and shape by consolidation, often by simply pressing nominally dry powder. Ceramic powders are commonly pressed in steel dies or rubber bags with the aim of producing a near-net-shape green body for subsequent sintering. Density gradients in these compacts, introduced during the pressing operation, are often severe enough to cause distortions in the shape of the part during sintering due to nonuniform shrinkage. In such cases, extensive green machining or diamond grinding may be required to produce a part with the desired final shape and size. In severe

cases, density gradients and nonuniform shrinkage may even create cracks in the parts during sintering. Likewise, severe density gradients can result in green bodies that break during ejection from the die or that are too fragile to be handled during subsequent processing.

While empirical relationships (i.e., rules of thumb) exist to describe powder compaction, they do not provide the understanding necessary to control die design or compaction parameters to eliminate density gradients; consequently, the designer is forced to use expensive and time-consuming trial and error procedures to develop new components. The problem with this traditional approach is that compaction density gradients of unknown and uncontrolled magnitude are inevitably introduced in the process, contributing to warping and uncontrolled sintering, and ultimately to unpredictable component performance and reliability. For this reason, interest has grown in developing and applying computational tools to address the problem [1,2].

The technical approach that we have taken in this work has been to apply fundamental scientific understanding to develop an overall predictive model for powder compaction. A scientifically-based model should help us to design cost-effective processes to manufacture improved performance and reliability ceramics by providing the insight needed to control die design and/or compaction to minimize density gradients. The objective of this work, therefore, has been to develop an overall predictive model for powder compaction that will aid in producing components of accurate shape and size, as-sintered, without the need to perform extensive machining. We call this a “model-based design and processing” approach.

Development of our macroscopic, continuum-based, FE technology has involved four distinct steps:

- We identified and further developed a mathematical material description (i.e., constitutive model) capable of predicting ceramic powder consolidation response in the form of a multisurface plasticity model that is typically referred to as a cap-plasticity model [3];
- We identified, extended, and implemented a testing methodology to characterize ceramic powders in a manner consistent with the mathematical description to estimate parameters for the constitutive model;
- We implemented the constitutive model within a more general-purpose, established, and accepted numerical simulation technique (i.e., the finite element method, FEM) as embodied within the nonlinear, inelastic, large-deformation FE program, JAS3D [4]; and

- We validated the predictive capability afforded by the overall model to ceramic powder compaction.

The resulting tool is a powerful, predictive tool for ceramic powder compaction.

Beyond this, we also developed specialized software that wraps around various tools from Sandia's FE toolkit, including the more general-purpose software. The specialized software targets a general subclass of axisymmetric compacts, typical of many commonly pressed parts. Its purpose is to provide a user-friendly, simple interface to the various tools in the FE toolkit that are typically needed to perform an analysis and to visualize/interpret the results from the FE analysis within the context of ceramic component manufacturing.

This paper will describe and discuss the details of each of the steps identified above to develop the underlying general FE technology and will delve into the specialized software that has been developed for nonexperts in the field of FE analysis.

CAP-PLASTICITY CONSTITUTIVE MODEL

Geotechnical engineers have had a rich and extensive history of providing tools to help evaluate soils behavior in the context of soil-structure interaction, a process that is analogous to the interaction of a ceramic powder with a metal die and/or rubber bag. For this reason, we began the search for a mathematical model of material behavior that might be applicable to ceramic powder compaction in the geotechnical literature. Among the many mathematical descriptions available, we sought one that could capture both the hydrostatic and deviatoric response of the powder; namely, one that could capture the compaction due to mean stresses (pressure) as well as the plastic flow and enhancement of compaction due to deviatoric stresses (shear). The justification for this is based on the analysis of a typical powder compaction curve obtained by uniaxial pressing relative to the measured density gradients in a die-pressed compact (Figure 1). The compaction curve in Figure 1a represents the average relative density obtained for a 94 wt% alumina body as a function of the applied compaction pressure. The fringe plot of relative density in Figure 1b was obtained by removing a central slice from a pressed alumina compact and determining spatial density using ultrasound velocity measurements. In this particular case, a 94 wt% alumina compact, 22.2 mm in diameter by 35.1 mm tall, was formed using a pressure of 68.9 MPa applied from the top. The highest relative density of 0.56 is measured in the upper right corner, as seen in the fringe plot. To reach such a compacted state implies that either the local

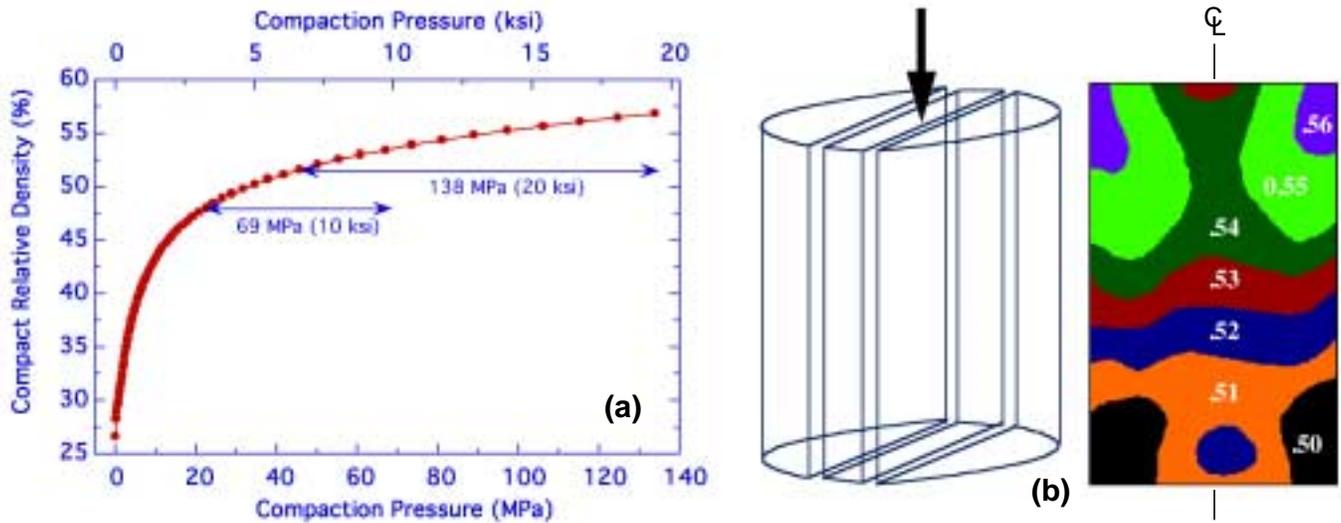


Figure 1: Measured (a) Powder Compaction Curve and (b) Density Gradients for a 94 wt% Alumina Compact Top-Pressed to 68.9 MPa.

“pressure” in that region was *significantly* higher than the applied 68.9 MPa or that the consolidation behavior of the powder is also influenced by the high deviatoric stresses occurring in that area due to friction between the powder and the die-wall. Because it is unlikely that higher pressure alone could account for the higher degree of compaction, a mathematical description of material behavior that allowed for the enhancement of compaction was deemed necessary.

A model that captures the mechanical behavior of granular materials during consolidation, allowing for this enhancement of compaction, is the “cap-plasticity” model of Sandler and Rubin [3], shown schematically in Figure 2. The ordinate in this figure is the first invariant of stress (three times the mean stress or hydrostatic

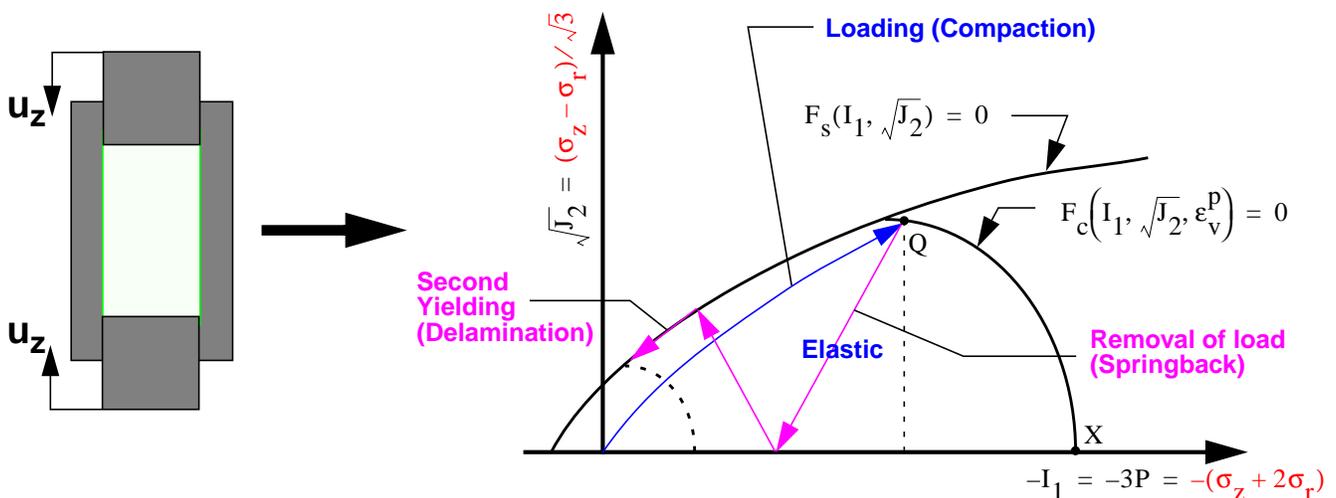


Figure 2: Schematic of Material Response Captured by Cap-Plasticity Model.

“pressure”) and the abscissa is the second invariant of the deviatoric stress (a measure of the shearing stresses). Features of this model include two yield surfaces, one a stationary shear failure envelope, F_s , and the other a non-stationary strain-hardening cap, F_c , that bound the elastic regime. This allows for an initially “small” cap that grows and hardens during loading (compaction), an elastic rebound upon unloading (spring-back), and the possibility for secondary yielding (delamination) if unloading results in an intersection with the failure envelope. In Figure 2, material subjected to a stress state “Q” located on the cap would undergo the same effective compaction that material subjected to a stress state “X” on the cap; however the compaction of material at “Q” would be enhanced by the deviatoric component beyond what could be achieved by the hydrostatic component alone. Effectively, it “appears” that the material at “Q” is subjected to the higher purely hydrostatic stress state at “X.”

The cap-plasticity model implemented and used in this work is a generalization of the Sandler-Rubin constitutive model. It was generalized so that it incorporates Lode-angle dependence of yield in the deviatoric plane and nonassociativity in the meridional plane on the shear failure surface. Details of this generalized model can be found in Argüello *et al.* [5]. The material model also includes a modified functional form of the pressure versus volumetric strain response to better-capture ceramic powder behavior.

The material parameters that define the surfaces and other pertinent characteristics of the model come from a combination of laboratory hydrostatic compression tests and from confined triaxial compression tests. Fossum *et al.* [6] have outlined the techniques by which hydrostatic and triaxial compression experiments are used to obtain parameters for models of the foregoing type.

CHARACTERIZATION OF CERAMIC POWDER MATERIAL RESPONSE

The 94 wt% alumina powder is comprised of nominally micrometer-size primary particles that has been granulated with organic binder through spray drying to produce nominally 100 micrometer agglomerates. After firing, the finished product is a debased alumina body comprised of alumina and a silicate-based glass phase. The designation for the powder signifies that 94% of the inorganic matter present in the green powder is alumina, and 6% is glass. Additionally, the powder contains several percent of organic matter, some of which is intentionally added as a binder to aid in forming and to provide the compacted powder (tensile) strength after

press forming. A theoretical green density of 3.54 g/cc is calculated from the constituents for the powder.

Hydrostatic compression experiments are performed to determine the evolution of the cap along the I_1 ($\sqrt{J_2} = 0$) axis, and to measure the bulk modulus at the pressure(s) of interest. The onset of permanent volume strain marks the initial location of the cap on the I_1 axis, and subsequent increases in pressure result in permanent hardening. The initial bulk modulus, and those of the hardened states, are measured by monitoring strains during small depressurization/repressurization cycles at the corresponding pressures [7].

Triaxial compression experiments are used for several purposes. First, they are used to locate the position of the shear failure surface in $\sqrt{J_2} - I_1$ space. The shear failure surface is usually (but not always) taken to be the loci of points in $\sqrt{J_2} - I_1$ space outside of which the specimen will no longer support increasing deviatoric loads. Second, during deviatoric loading, small unload/reload cycles can be performed to measure Young's modulus and Poisson's ratio for the corresponding stress state [7]. Finally, by overhardening the specimens with a hydrostatic pressure sufficiently great to cause permanent strain, and then dropping to a lower pressure before deviatoric loading, the off-axis shape and evolution of the cap can be probed: Deformation within the cap-failure envelope wedge is elastic; when the “new” cap is reached, permanent shear and volumetric strain begin to accumulate.

Knowing the bulk and Young's moduli, and Poisson's ratio, the shear modulus can be calculated. Thus, all required parameters for the model can be obtained from these two types of experiments.

Our experiments, described in more detail in Zeuch *et al.* [8], were performed using a standard, liquid-medium, triaxial cell [7]. The cell consisted of a cylindrical, 200 MPa pressure vessel with one end of the closure penetrated by a moveable piston. The piston permitted application of a deviatoric load to a test specimen concurrent with a separately controlled hydrostatic pressure. For triaxial testing, this cell was mounted in a servo-controlled, 979 kN-capacity MTS frame that permitted transfer of load from the frame to the specimen. The cell was equipped with electrical feed-throughs that permitted direct strain measurements using various types of transducers, in this instance, linear variable displacement transducers (LVDTs).

Loose ceramic powders have very high porosities, so strains are large and inhomogeneous even under hydrostatic compression. Direct triaxial compression experiments on such specimens would not be useful

because the initial state of the specimen (other than its density) would be poorly defined. For this reason, experiments on ceramic powders were conducted in two separate steps, which we call the hydrostatic and triaxial stages. In the first stage, the loose powders were compacted under a succession of hydrostatic pressures to establish pressure-density curves for each of the powders and to create a suite of pre-compacted specimens of known density and dimensions for the triaxial series. The specimen assembly consisted of a cylindrical, 44.5 mm inner diameter by 133.4 mm long Viton jacket, sealed with two aluminum endcaps fitted with O-rings. One endcap was vented to the atmosphere via a tube that penetrated the lower end closure to permit gas to escape from the specimen and test in the “drained” condition [7].

To prepare a specimen, a known weight of powder was poured into the rubber jacket-endcap assembly and vibrated for 60 seconds, followed by carefully assembling the vented endcap to the rubber jacket.

Volume measurements were then made on the assembly using Archimedes’ method. The known volume of the jacket plus endcaps was subtracted out to determine the volume and density of the powder. The assembled specimen was then loaded into the pressure vessel, and successively pressurized to several different pressures. At the maximum pressure for each pressurization stage, a vacuum was applied to the specimen to keep the rubber jacket compressed tightly against the powder and the sample was removed from the vessel. Volume measurements were then made on the compacted specimen, and a density corresponding to that particular pressure was determined. The sample was then returned to the pressure vessel, and the specimen was pressurized to the next value in the series, until the final (*target*) pressure was reached. Typically, our target pressures were 6.9, 20.7, 34.5, 51.7, and 68.9 MPa. In this way, we determined the pressure-density curves for the powders up to 68.9 MPa and also obtained a suite of pre-compacted specimens of known density that were subsequently machined into cylinders of known length and diameter for triaxial testing.

For triaxial testing, the hydrostatically pressed cylindrical specimens were jacketed in polyolefin tubing and sealed with endcaps, with the lower endcap again vented. The endcaps were equipped with holders for a pair of diametrically opposed LVDTs to measure axial strain. A single spring-loaded LVDT held in a clip-on fixture measured diametral strain.

This assembly was returned to the triaxial test cell, and pressurized back to the highest pressure that the

specimen experienced during the hydrostatic stage. Once the target pressure was reached, a depressurization/pressurization cycle was performed to measure the bulk modulus. The absolute magnitude of the pressure cycle depended on the target pressure, with larger loops possible at higher pressures. To preserve the original state of the specimen, it was never completely depressurized during the depressurization-pressurization loop.

For triaxial testing, the moveable piston was brought into contact with the specimen endcap and then moved at a constant displacement rate corresponding to a nominal axial strain rate of $1 \times 10^{-4} \text{ s}^{-1}$. During the course of the axial deformation, the specimen was partially unloaded and reloaded periodically to measure Young's modulus and Poisson's ratio. Again, the magnitude of the cycle depended on the confining pressure and strength of the specimen. Pronounced "barreling" of the specimens was observed under all test conditions, and axial stresses were continuously corrected for the change in cross-sectional area.

FINITE ELEMENT DISCRETIZATION

The cap-plasticity constitutive model described can be incorporated into simple mathematical algorithms to model specific simple geometries and compacts of academic interest; however, for application to problems that are of interest to ceramic component manufacturers, a much more general tool was needed. Realistically, a useful tool has to be able to capture the varied and complex geometries of real pressed parts; the general loading and unloading conditions that are imposed when those parts are manufactured; and the general initial and boundary conditions that must be imposed to yield a desired part. A general-purpose, established, and accepted numerical simulation technique that provides this functionality is the finite element method. In particular, the advanced quasistatic FE technology developed by Sandia National Laboratories that is based on iterative solvers has been a key element in our program. This technology has been specifically and extensively developed under defense programs to handle large problems involving large deformations, exactly the type of problem typically encountered when simulating the pressing of ceramic components. The use of iterative solvers and the extensive experience with non-linear material response that exists at Sandia provided a base technology that offered an efficient solution to this type of problem.

For the displacement-based FEM used in this work, the field equations governing deformation of a body can be discretized and written as [5]:

$$\left\{ \sum_N \int_{ve} \mathbf{B} \boldsymbol{\sigma} dV \right\} = \{\mathbf{F}\}, \text{ or } [\mathbf{K}(\mathbf{u})] \{\mathbf{u}\} = \{\mathbf{F}\}, \quad (1)$$

where the term on the left-hand side of each form of the equation is the internal force vector, and $\{\mathbf{F}\}$ is the external force vector. In the first form, \mathbf{B} is the strain-displacement transformation matrix, N is the number of elements in the FEM discretization, $\boldsymbol{\sigma}$ is an ordered vector of stress components in each element at a Gauss point, and ve is the volume of each element. In the second form of Equation (1), on the right, $[\mathbf{K}(\mathbf{u})]$ represents the global stiffness matrix in the traditional FEM [9] and $\{\mathbf{u}\}$ represents the global vector of unknown nodal displacements. Both forms of the equation are included to highlight the differences in approach between the traditional FEM approach and the explicit approach used in this work within the quasistatic non-linear FE program, JAS3D [4]. The stress-strain relationship (constitutive model) is incorporated via the integrand product in the left-hand side of the first form of Equation (1) and is similarly incorporated within the left-hand side of the second form as well. The cap-plasticity constitutive model described above was implemented within JAS3D in the form of a material subroutine and constitutes one of many material models available in the code for simulating various advanced industrial processes.

The explicit technology that forms the basis of the present work approaches the solution of Equation (1) in a manner different from that used in the traditional FEM [9]. First, a global stiffness matrix is never formed. Instead, at the element level, the divergence of the stress is found, and the contributions to each node in the overall structure are summed (i.e., the vector described by the left side of the first form of the equation). A residual force vector comprised of the internal minus the external forces,

$$\{\mathbf{R}\} = \left\{ \sum_N \int_{ve} \mathbf{B} \boldsymbol{\sigma} dV \right\} - \{\mathbf{F}\}, \quad (2)$$

is computed, and the solution procedure is then one of reducing the residual to zero using an iterative technique. Because the quantities being manipulated are vectors, there is no need to store a global stiffness matrix and factor it. Consequently the storage requirements are small when compared to the traditional FEM approach and larger problems can be solved more efficiently. The two iterative techniques that are currently used in JAS3D are a pre-conditioned Conjugate Gradient (CG) technique [10] and an adaptive Dynamic

Relaxation (DR) technique [11].

MODEL VALIDATION FOR SIMULATING POWDER COMPACTION

Once the cap-plasticity model was implemented within JAS3D, confidence needed to be established in the accuracy of the overall model for predicting powder compaction response. Although JAS3D continuously undergoes many specific processes to improve software quality (e.g., change control, configuration control, regression testing, etc.), its predictive capability using the newly implemented constitutive model needed to be ascertained.

The first check performed was to simulate one of the laboratory tests performed on the 94 wt% alumina. The triaxial test at 68.9 MPa confining pressure was chosen and the entire loading history of the material was simulated, i.e., hydrostatic loading to target confining pressure followed by an increasing axial load thereafter. The simulation was performed using the material parameters obtained from all the hydrostatic and triaxial tests completed on this specific powder. Figure 3a shows the results of the JAS3D simulation overlaid on the data from the laboratory experiment. Axial stress is plotted as a function of the axial and radial components of strain. With the obvious exception that the JAS3D simulation did not include any of the unload/reload cycles seen in the data, the figure shows that there is good agreement between the simulation and the experiment. During the phase of hydrostatic loading to the target confining pressure of 68.9 MPa, all components of strain are equivalent. However as the axial stress increases beyond the confining pressure, during the actual triaxial phase of the test, the axial strain continues to increase while the radial strain begins to decrease. In both the simulation and experiment, the maximum value of axial stress reached is about 172.4 MPa.

With confidence that the cap-plasticity model had been implemented correctly within JAS3D, a more complex simulation was performed. The uniaxial compaction of the cylindrical specimen shown in Figure 1b was undertaken assuming a compaction ratio of about 1.9 (i.e., the powder fill height was 67 mm). This is more complicated because we have to account for the interaction of the powder with the die-wall. The contact interaction in JAS3D was modeled simply with Coulomb friction and the coefficient of friction between the die-wall and the powder was assumed to be 0.2, which is in the range of values measured for the interaction of ceramic powders with various die-wall materials. Because of symmetry and an assumption of uniformity in

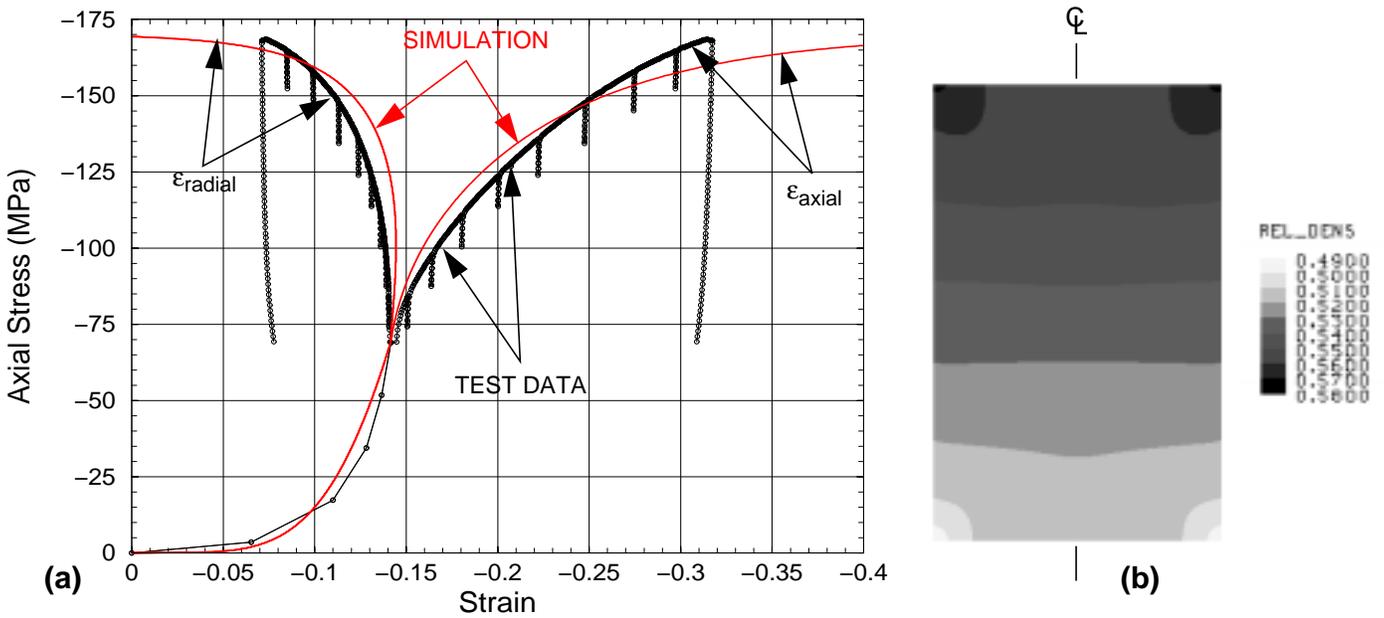


Figure 3: (a) Comparison of Data from Confined (68.9 MPa) Triaxial Compression Test with a JAS3D Simulation (b) Fringe Plot of Computed Relative Density for the Uniaxially Compacted Cylinder in Figure 1b.

die-filling, only a wedge of the cylinder needed to be modeled with JAS3D. The fringe plot of computed relative density from this simulation is shown in Figure 3b. The computed relative density at the outer top of the compact is 0.56- 0.57, while that at the outer bottom is 0.50-0.51. These predictions compare quite well with the respective measured values of 0.56 and 0.50 in Figure 1b. The spatial distribution of relative density, however, is somewhat different, particularly in the radial direction near the top and bottom of the cylinder. This may be attributable to several things, among them the manner in which the upper and lower boundaries were specified in the simulation. In the simulation, material was free to move radially but not axially relative to the vertically moving boundary at the top and the stationary boundary at the bottom. In the real pressing scenario, there are platens at the top and bottom that also interact with the powder and will induce shearing stresses. Furthermore, a uniform die-fill was assumed in the simulation that is undoubtedly not the case in the real part: this can be inferred by the presence of asymmetry in the density distribution relative to the axis of the cylinder in Figure 1b. Finally, the coefficient of friction between the die-wall and the powder may be different from the assumed value, or the frictional interaction may not be simple Coulomb friction.

Additional simulations have been performed on more complex geometry compacts to gain further confidence in the predictive capability of the overall model, and we have had a similar degree of success in predict-

ing density distributions. Ultimately, however, the real test of the model's predictive capability will be at the hands of ceramic component manufacturers who must gain confidence in this tool by comparing code predictions with measured data from a wide range of production parts.

SPECIALIZED SOFTWARE

The resulting tool above can be used to predict forming stresses, density gradients, and material flow to investigate the effects of compact geometry; compaction ratio; pressing conditions (single, dual, hydrostatic pressing); die-wall friction coefficient; and die design (tapers, corner radii, etc.). As such, it constitutes part of the general underlying software, that we will refer to as the Sandia FE "toolkit" that is available to model even the most complicated 3D ceramic compacts envisioned. Effective use of the software at this level, however, requires significant FE modeling expertise, insight into the underlying mechanics of the compaction process, and experience in using the cap-plasticity constitutive model and the JAS3D code. Furthermore, constructing the FE mesh that is part of the required input to JAS3D as well as visualizing results from the database output from JAS3D depends on several additional pre- and post-processing tools from the toolkit.

These significant requirements and potential impediments for using the underlying software, by the typical engineer on the production floor, called for a more user-friendly tool than the general-purpose capability described. To achieve this goal, it became essential to limit the scope of the class of problems to be handled by the software without being overly restrictive. The flexibility to model simple and complex geometry was achieved by developing higher-level specialized software to wrap around the general toolkit to address geometry variability within the axisymmetric subclass of compacts that are quite common in the industry.

This was accomplished by allowing multiple concentric cylinders to be stacked axially, as depicted schematically for three cylinders in Figure 4. The cylinders are interconnected using smaller transition radii that can be varied systematically. The individual cylinders, which can be solid or hollow, are allowed to have variable inner and outer diameters and heights. By linking the different size and shape cylinders axially, it is possible to model geometric features like counter-bores and bushing stems that are common in complex-geometry ceramic components fabricated by powder pressing. In addition to the geometric variables mentioned, the software also provides some capability to realistically vary the properties of the die and powder

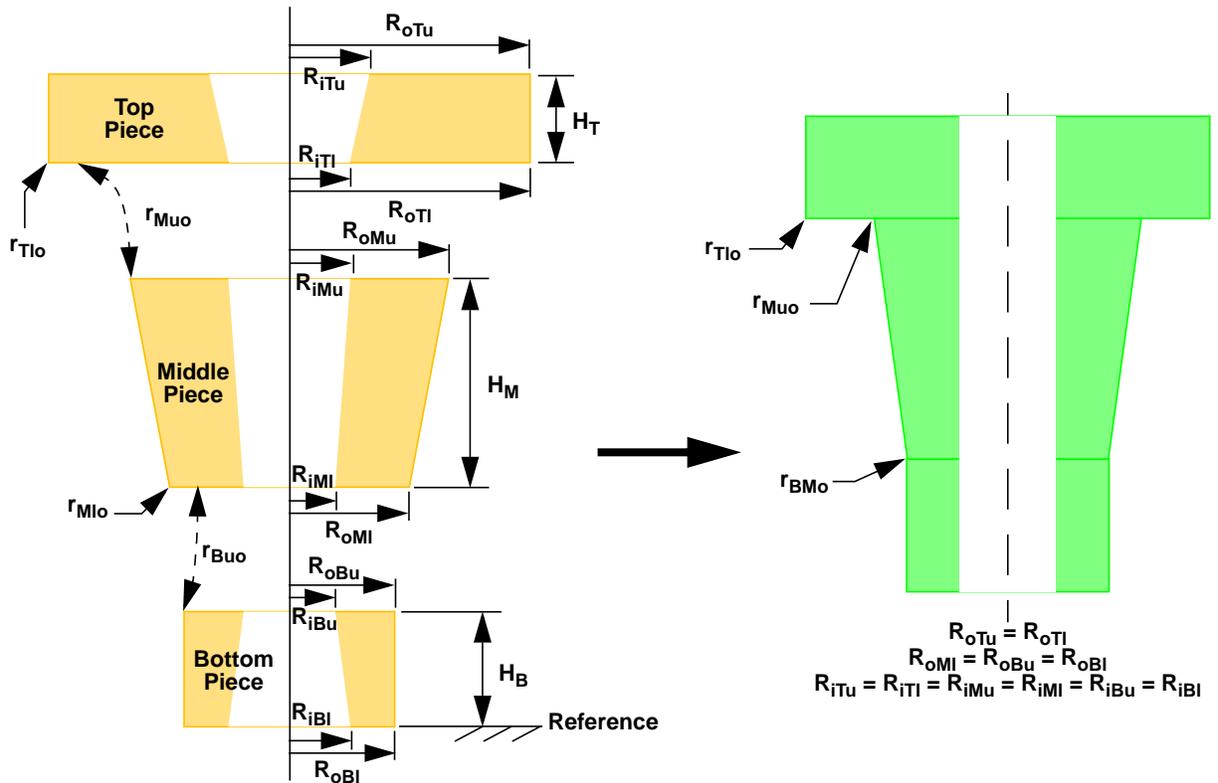


Figure 4: Schematic of a Complex Part Built Up from Three Stacked Axisymmetric Pieces.

compact materials, as well as the loading applied to the compacts.

At the heart of the software we call “UNIPACK” is a top-level driver that queries the user, builds and parses input parameter files, and wraps around Sandia’s existing FE analysis toolkit to automatically perform a ceramic powder compaction analysis. In addition, there are key, pre-built files that contain the logic to generate the mesh for the compact in question from the input geometric quantities.

The overall flow of the specialized UNIPACK software package is depicted in Figure 5. There are three distinct phases that are automatically handled by the software:

- Geometry Definition Phase – Queries user for geometry information, builds user parameter files, and parses these files to the FE pre-processing tools to build the FE mesh for use in the analysis.
- Run Definition Phase – Queries user for parameters that define pressing conditions and type of material (specific powder) being pressed; builds a file of user parameters, and parses this file to a pre-processing tool to build an input deck for JAS3D.
- Solution & Post-processing Phase – Submits the FE analysis run; after the analysis finishes, it calls the FE post-processing tool to query the FE results database and generates a postscript file of select results; it

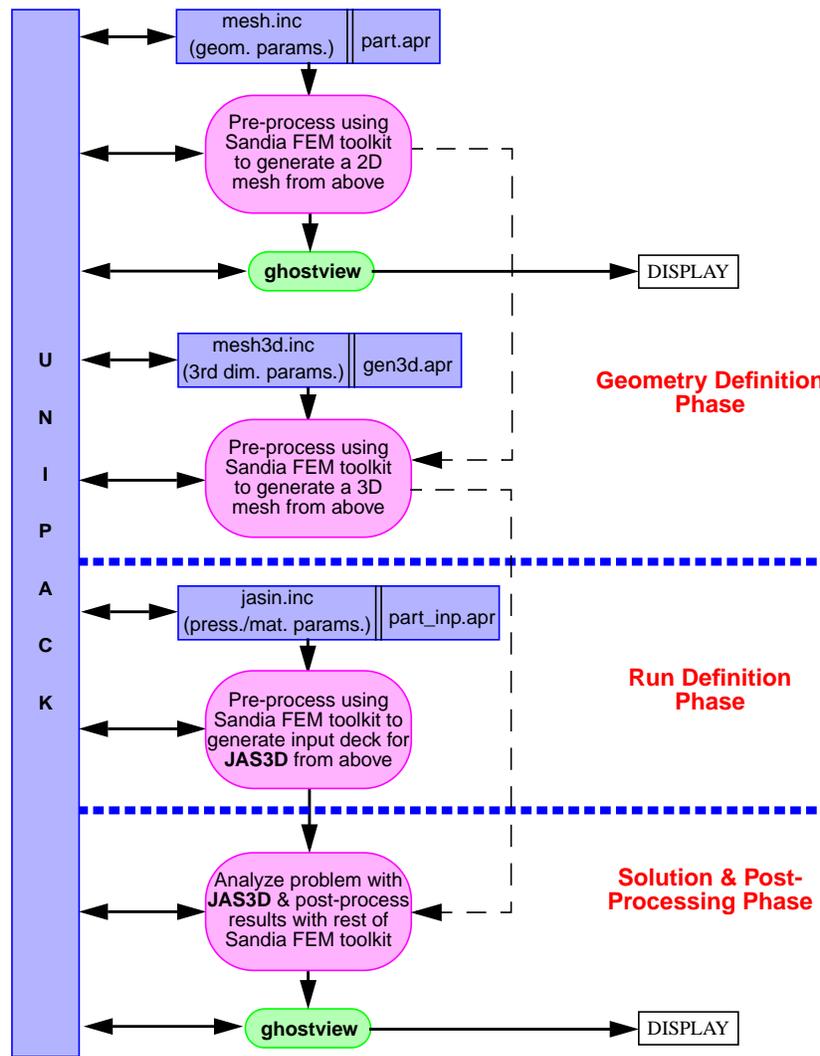


Figure 5: Flow Diagram Depicting How Unipack Drives and Wraps Around Existing Tools from the Sandia Finite Element Toolkit.

then launches a postscript viewer to display this file to the user.

Thus, the expertise required to build the input deck, run the FE analysis code, and post-process the results resides in the specialized package. The user simply responds to a series of prompts, evaluates the quality of the FE mesh that is generated automatically, and analyzes the graphical results generated from the simulation. Figure 6 shows a two-piece part simulated with the specialized software. Figure 6a is a schematic of the problem, showing that very few parameters are needed by the software to perform the simulation (ten radii, two heights, etc.). Figure 6b is an actual postscript image of results from the simulation that is presented to the user at the end of the simulation. In this case, it is a fringe plot of relative density; i.e., relative to the starting density. This relatively small simulation takes about 30 minutes of CPU time to run under the Linux OS on a

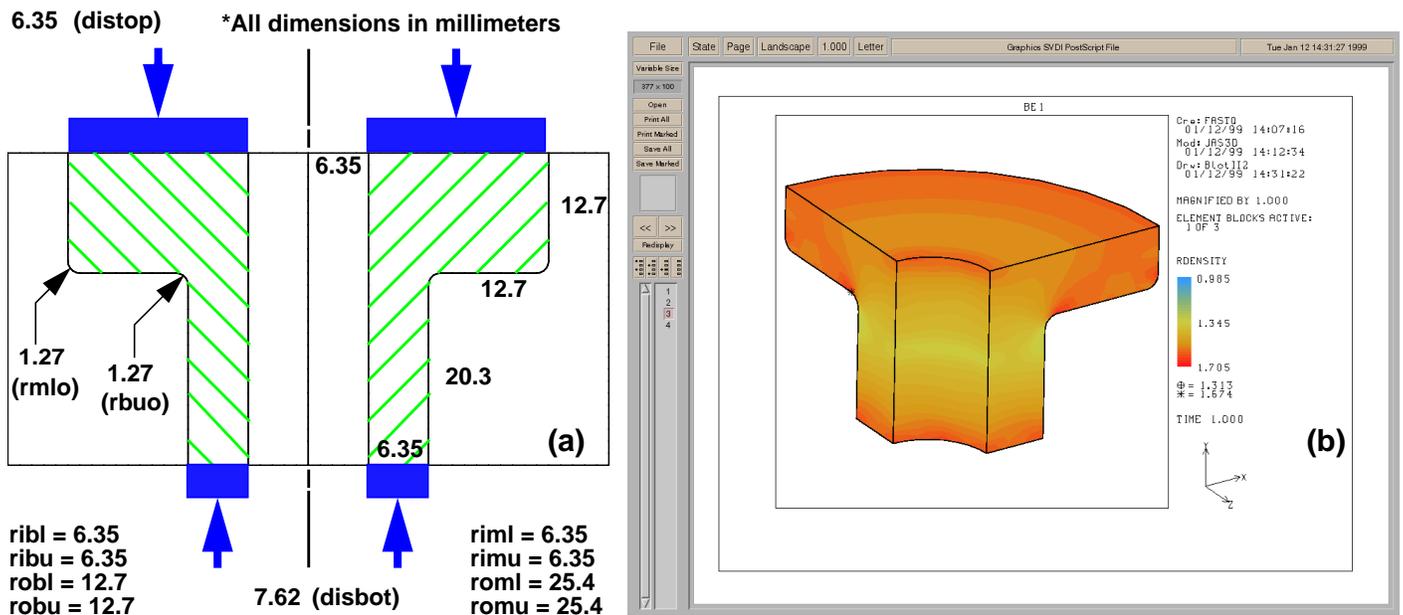


Figure 6: Sample Two-Piece Compact Simulated with Specialized Software (a) Parameters Needed by Package (b) Postscript Image of Density Fringe Plot from the Simulation.

450 MHz Pentium III PC.

This specialized software tool allows users with little or no FE expertise to benefit from the tremendous power and insight that FE analysis can bring to the design cycle. Furthermore, as the user develops expertise in modeling the powder compaction process with the specialized software package, the more general underlying software is available to him to allow modeling of more complicated geometries and processes.

SUMMARY AND CONCLUSIONS

A cap-plasticity constitutive model, originally developed to predict the geomechanical response of soils, has been adapted to simulate the compaction of ceramic powders. The parameters for the constitutive model are obtained from an extensive suite of hydrostatic and triaxial compression “soils-like” laboratory tests on specific ceramic powders. The constitutive model has been implemented in a finite element program for simulating the quasistatic, nonlinear, large deformation, inelastic response of solids. The overall tool has been used to predict and investigate the response of different powder compacts to various die-design details and parameters and pressing conditions. Thus the overall model has been at least qualitatively validated for ceramic powder compaction, and additional efforts are underway to further exercise and obtain increased confidence in its predictive capability.

Recent efforts have focused on developing a “user-friendly” powder compaction “package” in which the “expertise” required to perform the highly nonlinear analyses on a subclass of axisymmetric “complex” parts is embedded within the system and invisible to the user. A “test-of-concept” version of the software package for die-pressed compacts, running under Linux on a PC, has been demonstrated and was released to our industrial partners. In turn, they will exercise the specialized software; compare its predictive capability to production parts; and suggest improvements for the package. Generalization of the specialized software to include biaxial-pressing and bag-pressing is also currently underway.

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