Modeling and experimental investigation of fracture behavior of pharmaceutical powder compacts

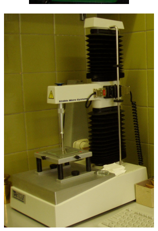
Ozgur Keles, Edwin García, Keith Bowman
Purdue University, West Lafayette, IN
School of Materials Engineering

Abstract

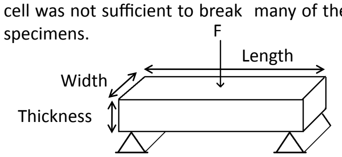
Experimental determination of green body strength is routine for pharmacy, powder metallurgy and ceramic industries. However, the pharmacy industry is responsible for development of new active materials with unknown properties. In this respect, the aim of this study is to understand the microstructural effects on the fracture behavior of materials and build a computer model to predict these effects with a special emphasis on automation of pharmaceutical powder processes and particle size after compaction and granulation. Three and four point bending tests, hardness and compression tests together with x-ray, optical and SEM investigations are the primary experimental aspects of the characterization. The resulting data from the experiments are used as a basis for a computer model to predict the fracture behavior of materials. This model for fracture will be applied to milling of roller compacted materials and compaction of milled powders, including phenomena such as capping [1]. Finite element and discrete element methods are primarily used for simulations.

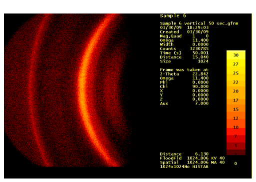
Experimental Approach

Avicel PH105, PH101 and PH102 microcrystalline powders were uniaxially compacted using an automated hydraulic Carver press and a rectangular die set. Various compaction forces were used to get different vol.% compacts.



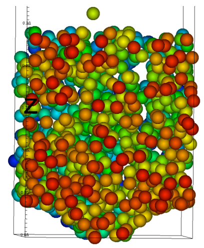
Three point bend tests were done by a Texture Analyzer TA XT. Same setup were also used for indentation tests but the load cell was not sufficient to break many of the specimens.



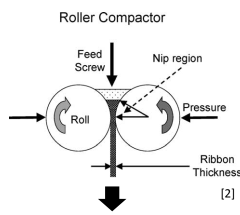


A Bruker general area detector diffractometer system (GADDS) was used to see mechanical texture in the powder compacts. There is not a strong texture; however, expected density variation was observed through the thickness.

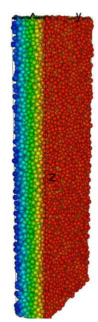
Modeling approach



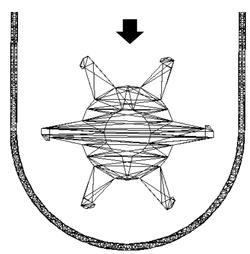
Discrete element method (DEM) has been used for modeling granular systems and fracture behavior of soil, asphalt and rock[3, 4]. In this study LIGGGHTS program[5] was used and particle interactions are based on Hertzian contact model. Different particles and size distributions with cohesion can be used for observing mixing, agglomeration and flow behavior of pharmaceutical materials.

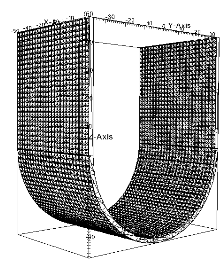


Roller compaction process can be simulated via DEM. Lack of extensive plastic deformations is the limiting factor in having high density compacted materials. However, particle properties like Young's modulus, Poisson's ratio and surface energy can be adjusted to have a similar bulk response of deformed particle compacts.



Various milling techniques and sieve types can be simulated by importing related mesh geometry. Effect of ribbon feed speed, mill speed, hammer geometry, sieve position and size on final particle size and distribution can be investigated. Flow properties and compaction of granules can be simulated to predict final tablet properties.



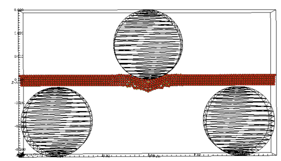


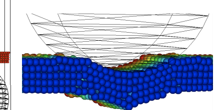
Model Validation

3-point bend test simulations:

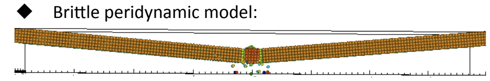
- Cohesive hertzian model:

The aim of the 3-point bend test simulations is to validate fracture behavior by comparing simulation and experimental results. Cohesive Hertzian model was used to generate a ribbon of simple cubic packed particles. 3-point bend test was done to see the mechanical response and fracture behavior of the ribbon.

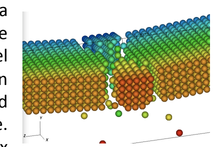




- Brittle peridynamic model:

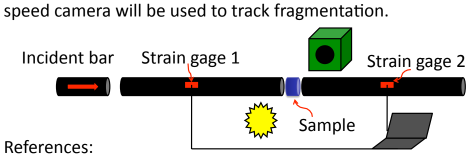


LAMMPS molecular dynamics code was used to test a peridynamic brittle solid [6]. Some of the advantages of this model are directional bonding, built-in strain based fracture criteria and no bond formation after fracture. However, there is not any complex wall interactions and particle size distribution.



Future Work

Split Hopkinson bar will be used to see the effect of high strain rate on fracture behavior of compacted powders. High speed camera will be used to track fragmentation.



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