Elastoplastic Response of Compacted Pharmaceutical Powder Blends: Model Development, Calibration and Validation

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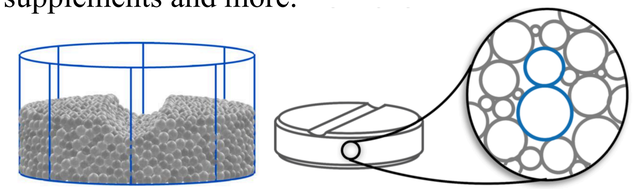
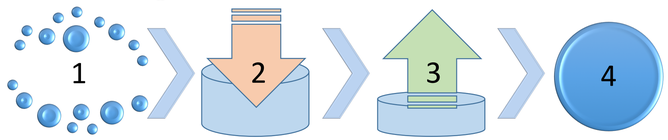
Background and Introduction

Compaction of powders is a common process for industrial farming, pharmaceuticals, diagnostics, supplements and more.



A mixture is turned into a single bonded compact (tablet) by the application of compressive forces in four stages:



Die Filling | Compaction | Unloading | Ejection

Particles undergo elastic and plastic deformation, leading to bond formation

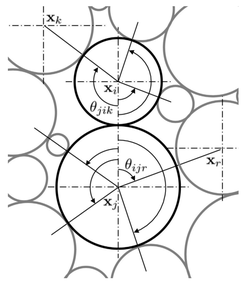
The compact experiences elastic relaxation after it is plastically deformed

Objectives

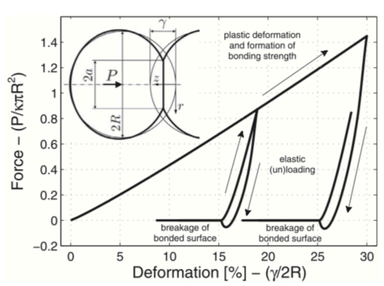
- As product performance of compacted particles depends on their microstructure, we seek to better model how these properties manifest at the continuum level.
- Our objective was to update the nanoHUB Powder Compaction tool, to include a model of elastoplastic response during unloading stage.

Methodology

The tool applies a particle mechanics approach to model the compaction process using generalized loading-unloading contact laws for elastoplastic spheres with bonding strength[1,2].



[1]



[2]

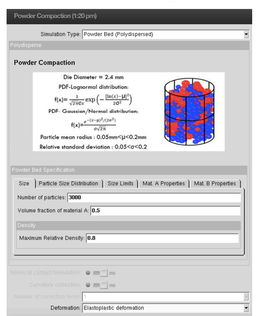
Gamlen Tablet Press

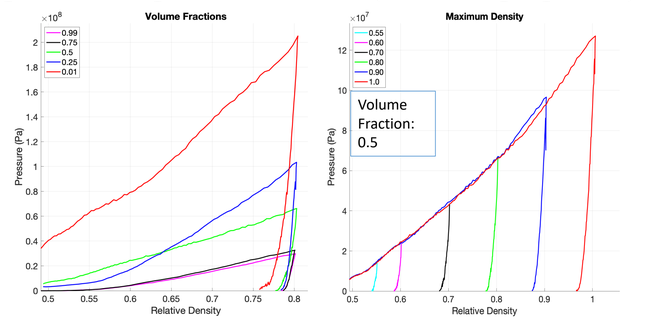
Experimental data was obtained with a benchtop tablet press that was used to calibrate and validate the model. The powders used were Microcrystalline Cellulose (MCC) and Lactose.

nanoHUB Powder Compaction v5.0

The new version (https://nanohub.org/tools/gscompaction) includes:

- User defined target relative density for the unloading point.
- Mixture of polydisperse elastoplastic materials (PDS and properties).

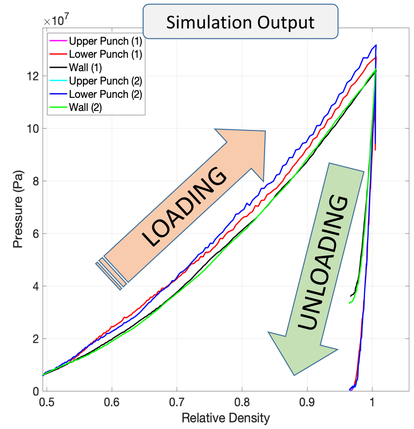


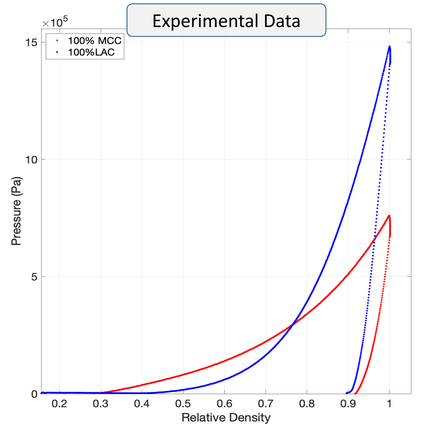


	Min Radius	Max Radius	Distribution	Young's Modulus	Poisson's Ratio	Plastic Law Stiffness	Inverse strain hardening exponent	Fracture Toughness
Powder A	0mm	0.3mm	Log Normal	5GPa	0.25	150MPa	2	1.26
Powedr B	0mm	0.3mm	Log Normal	30GPa	0.25	900MPa	2	6.19

➢ 0.75 Volume Fraction = 75% Powder A and 25% Powder B

Calibration and Validation





Verification of the Tool:

- Output from the tool is compared with output from the research code

Calibration of the Tool:

- Loading curve is used to calibrate plastic properties
- Unloading calibrates elastic and fracture properties

Conclusion and Future Work

The tool provides a better understanding of the underlying mechanics of compaction. Seamless integration of experimental and computational methods can augment development in the powder compaction field.

References

[1] Gonzalez, M. and Cuitiño, A.M. "Microstructure evolution of compressible granular systems under large deformations". *Journal of the Mechanics and Physics of Solids* 2016, **93**, 44-56,

[2] Gonzalez, M. "Generalized loading-unloading contact laws for elasto-plastic spheres with bonding strength". *Journal of the Mechanics and Physics of Solids* 2019, **122**, 633-656.

[3] Chen Shang; Yuqi Fang; Carlos E Fernandez-Caban; Wentao Chen; Ayush Giri; Caroline Baker; Yasasvi Raghavendra Bommireddy; Ankit Agarwal; Marcial Gonzalez (2017), "Powder Compaction," https://nanohub.org/resources/gscompaction

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