



IFPRI Project Abstract

[Project Title] Air-induced defect formation during powder compaction

Ken Kamrin

MIT and UC Berkeley, Mechanical Engineering

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Project Objective:

The focus of this project is to understand the physical mechanisms that lead to defect formation – pitting, cracking, and delamination – during pharmaceutical tableting. A leading hypothesis among IFPRI members is that trapped interstitial air leads to high pore pressures that tend to fracture adhered particle interfaces after removal of the confining pressure. The project objective is to explore this problem through coupled numerical methods including: (i) continuum mixture models and (ii) the discrete element method (DEM) coupled with a fluid solver.

Approach:

The primary barrier is the fact that the behavior of cohesive powders is not well understood, with neither a generally accepted constitutive relation nor contact model in existence. As such, the initial phase of the project develop a novel mechanically-derived cohesive powder contact model for usage in DEM. The completed contact model was published in the premier solid mechanics journal, *Journal of Mechanics and Physics of Solids*, as a two-part series. The contact model has been implemented as a custom DEM code in LIGGGHTS and LAMMPS, with the LAMMPS version being openly available. Using these implementations, our powder DEM capability has been shown to reproduce the multi-directional tableting stresses seen in a real experimental compaction simulators; no post-calibration was needed.

Recent Results:

Very recently, we have coupled our elastic-plastic contact model to a compressible gas phase to allow a complete, microscopic view into the process of defect formation in tableting. This was achieved by combining the multi-particle collision dynamics method (MPCD) for the gas phase with our discrete element powder method for the grains, as two mechanically interacting media within LAMMPS. Preliminary results show that the gas has a noticeable qualitative effect on the tablet formation and integrity, and in particular that stroke speed can affect defect formation in tableting. Gas pressure within the tablet can cause catastrophic expansive stresses upon tablet ejection.

Next Steps:

If renewed, our project will complete our verification of the air-powder simulation method and construct a diagrammatical map to instruct combinations of procedure and powder properties that can lead to tableting defects. We will validate against experiments of tableting run at different stroke speeds. We will use the air-DEM method as a digital twin to calibrate and implement a two-phase continuum model for tableting.
