



IFPRI Project Abstract

Air-induced defect formation during powder compaction

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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 project developed 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. Our recent goals have been to show this contact relation can be used in a DEM code to represent tableting accurately and to mix this method with a gas phase.

Recent Results:

- Our work on DEM simulation of tableting using our new contact model was just published in *Powder Technology* with IFPRI industry members as co-authors.
 - Our DEM method has been formally integrated into the LAMMPS default installation with full documentation.
 - We have coupled our powder contact model to a compressible gas phase to allow a complete, microscopic view into the process of defect formation in tableting. This is achieved by combining an MPCD model for the gas within our DEM powder method as two mechanically interacting media within LAMMPS.
 - Without air, we rarely encounter defect formation on ejection. However, with air we can see clear laminar defects form. The defects are influenced by air in a manner that matches air playing a large role; more defects when increasing the air viscosity and fewer when the relative density of the tablet is lowered.
 - We are also assisting other IFPRI members in using our new code for other powder processing problems such as pelleting.
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Next Steps: 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.