IFPRI Project Abstract

[Project Title] Air-Induced Defect Formation During Powder Compaction

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Project Objective:

This project aims to understand tableting fracture defects and in particular to determine the role that air may play in triggering fractures during the tableting process. The goal is to first produce a CFD-DEM simulation capability that includes a novel powder DEM method based on elastic-plastic particle contacts with JKR-like adhesion. This method can be used to simulate tableting, and we can dissect its results to determine the role of the air. This method can then be used to guide a two-phase continuum approach to simulating the tablet compaction process, which can be implemented using the PI's existing meshless techniques.

Approach:

The approach to developing this method is multi-part. The novel DEM method is primarily a theoretically-derived reduced-order approach based on bulk elasto-plasticity. This will be incorporated within Open-FOAM and LIGGGHTS to run CFD-DEM simulations of the tableting process, where we can check how die speed influences the likelihood of fractures, or conversely whether the fractures form independent of the presence of air (say, due to residual elastic stresses in the power grains). The discrete simulations will then be used to perform one-element tests that will allow us to calibrate the two-phase continuum mixture model; in particular the compaction "cap" yield surface for the solid (powder) phase and the packing-fraction-dependent drag relation for the gas-grain interaction.

Recent Results:

Over the last year, we have fully validated our new DEM approach (the so-called "MDR contact model") for multi-contact compaction of elastic-plastic grains through the entire range of limits, from the elastic range to the fully-plastic to the bulk elastic compaction regime. The scheme has also been verified to correctly capture unloading and adhesion between powder particles, both key to simulating potential fractures in tableting. In parallel, the DEM code is now being brought into the Open-FOAM package where it is being integrated into the CFD-DEM framework and used to simulate tablet compaction.

Next Steps:

Next year will focus on parameter studies of tablet compaction using CFD-DEM to determine the role of air in the failure process and to determine recommended practices to reduce tablet failures. In parallel, we will conduct a continuum extraction study to determine the bulk yield surface of the powder and couple this within a two-phase model, which can be run in a tableting geometry with a seed inhomogeneity to see if we can predict tablet failures from a continuum perspective.