IFPRI Brief Template

Check One: ☒**Project** ☐**Review** ☐**Collaboration** ☐**Workshop** ☐**Other**

Descriptive Title	Prediction of air-induced defect formation during powder compaction, via a multi-phase modeling framework that couples the evolution of solid structure with air permeation dynamics through the porous structure
Working Title[1]	Air-induced defect formation during powder compaction
Technical Area[2]	**F = Particle Formation**, M = Modeling
Date	25-Jun-2019
Short Description	A high-speed tableting process not only results in large deformation and strength development of the powder compact, but also can give rise to pore pressure buildup due to incomplete air escape through the closing pores. If the compaction happens too fast, the buildup in air pressure can be comparable to the strength of the compact and hence cause defects in the solid structure. This work aims to develop a novel air-solid coupling framework to quantitatively understand the above phenomenon. It will systematically study the effect of air flow / permeation on the strength development and defect formation of powder compacts. It builds on prior IFPRI efforts on compaction modeling (Zavaliangos, 2018 project) and pore-scale transport modeling (Cnudde, 2014 review), but will offer a brand-new perspective that integrates the dynamics of highly-compressible fluid and porous deformable solid, hence expand our capability to predict air-induced tableting failures. With such framework, insights into the formation of heterogeneities, anisotropies, and defects in the powder compacts can be explored. Further, modeling-based process optimizations to avoid air entrainment and associated defect formation can be achieved.
Objectives	1. Review of the current states in experimental, theoretical and simulation efforts on the interaction between evolving particulate structures, especially those under large deformations, and the air/fluid flow through their porous networks. 2. Develop (theoretical or simulation) framework that dynamically couples the deforming powder bed with the

[1] Title used in meeting agendas and file archives
[2] One or more from the following list: W = wet systems; D = dry systems; F = particle formation; SR = size reduction; M = modeling; SE = systems engineering

	associated air permeation. Construct local 3D constitutive relations to be used in industrially-relevant contexts (e.g., particle sizes/properties, die/punch geometries, compaction paths) for defect prediction. 3. Explore ways to incorporate select factors to better resemble realistic systems. Examples of such factors include: polydispersity, particle morphology, surface roughness, visco-elasticity, material mixture, etc. 4. Derive predictive tools to assess the risk of processing failures and aid optimization of the powder compaction process. Allow for cross-validations against experimental results.
Scope	• Included in scope: evolution of particulate structures under compaction, especially with large system-scale and particle-scale deformations; development of compact strength through particle bonding/adhesion; characterization of porous structures and the related air permeation behaviors; coupling between the solid structure evolution and air dynamics in the porous structure. • Representative material properties that align with IFPRI interest will be included in the scope. The simulation framework should be amenable to experimental verification/validation. • Considerations of the following and incorporation of them into the model will not be required but certainly encouraged: polydispersity, particle morphology, visco-elasticity, material mixture, particle breakage, particle surface interactions, etc.

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