

IFPRI Project Brief
Predictive Framework for Multicomponent Powder Compact Strength

Room temperature (“cold”) compaction of multicomponent powders is a commonly used operation to produce monolithic compacts with prescribed shape and a multiplicity of physical or performance characteristics, such as effective diffusivity (ceramic membranes), pore size (catalysts), disintegration rate (pharmaceutical or detergent tablets), burn rate (propellants), etc. In all cases, the compact must have sufficient tensile strength to survive subsequent processing, packaging, transport, and use.

The desired functionality of these compacts is commonly achieved by addition of specific “functional components”, and this often leads to highly complex, multicomponent formulations. In the absence of a suitable model for compaction of multicomponent mixtures, industrial practitioners are forced to resort to empiricism, making mixtures and measuring compact strength, which can lead to expensive (and incomplete) exploration of the formulation space and increased risk in development.

Thus, the objective of this project is to develop a predictive framework for strength development in multicomponent powder mixtures undergoing cold compaction at compaction stresses large enough to cause significant plastic deformation of particles. The model should be informed by and verified with experiments. More specifically, we are interested in semiquantitative prediction of strength as a function of composition, ingredient particle size distribution, and compaction pressure for an N-component blend ($N > 3$) which requires limited mechanical characterization of the individual components. This model should be based on micromechanics of compaction (e.g., the evolution of the texture of the developing compact and the contacts between particles). It should identify what particle-level properties and behaviors of single ingredients can be used to predict the cold-compacted strength of materials, answering the question of how industrially relevant particles fuse together to form high-strength compacts.

The project places no restriction on the multicomponent blends investigated (inorganic, organic, or metallic), but the blends must contain at least three components. Similarly, no restriction is placed on the compaction process, as long as the applied stress is sufficient to cause irreversible porosity loss.

Finally, statistical (AI) models are out of scope.