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Study of the die compaction of powders to high relative densities using the discrete element method

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Abstract

The mechanical behavior of powders during die compaction was investigated using the discrete element method (DEM), in which powders are modeled as discrete particles with elastoplastic material behavior. A new adhesive elastoplastic contact model that describes the force displacement behavior of contacting particles subjected to high confining conditions was introduced and implemented in DEM simulations of die compaction and uniaxial tension. The objectives of these simulations were: (1) to investigate the micromechanical behaviors of powder systems during die compaction; (2) to understand the influence of model parameters on the macroscopic behavior; and (3) to develop a methodology for the calibration of the model parameters from macroscopic experimental results. The methodology developed for the calibration of the model parameters was carried out by a combination of statistical design of experiments (DOE) and optimization techniques. The calibration methodology provided simulation results that were in good agreement with experimental results conducted on hot melt extruded (HME) copovidone powder. One of the key advantages of the calibration procedure is the need for only two experimental techniques – die compaction, and diametric compression strength tests. Furthermore, examination of the microscale behavior from simulated results revealed a connection between the level of interparticle cohesion and the corresponding level of residual wall stress of powder compacts after complete unloading in die compaction. It was found that lower levels of interparticle cohesion resulted in decreased residual wall stresses and an increase in the axial spring back from the minimum compact height at the end of compaction.

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