# Modeling of Pharmaceutical Tablet Compaction with Multi-Contact Discrete Element Method

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The purpose of this work is to simulate the powder compaction of pharmaceutical materials at the microscopic scale in order to better understand the interplay of mechanical forces between particles, and to predict their compression profiles by controlling the microstructure. For this task, the new framework of multi-contact discrete element method (MC-DEM) was used. In contrast to the conventional discrete element method (DEM), with MC-DEM interactions between multiple contacts on the same particle are now explicitly taken into account. A new adhesive elastoplastic multi-contact model invoking neighboring contact interaction was introduced and implemented. The uniaxial compaction of two microcrystalline cellulose grades (Avicel® PH 200 (FMC BioPolymer) and Pharmacel® 102 (DFE Pharma)) subjected to high confining conditions was studied. The objectives of these simulations were: (1) to investigate the micromechanical behavior; (2) to predict the macroscopic behavior; and (3) to develop a methodology for the calibration of the model parameters needed for the MC-DEM simulations. A two-stage calibration strategy was followed: first, the model parameters were directly measured at the micro-scale (particle level) and second, a meso-scale calibration was established between MC-DEM parameters and compression profiles of the pharmaceutical powders. The new MC-DEM framework could capture the main compressibility haracteristics of pharmaceutical materials and could successfully provide predictions on compression profiles at high relative densities.

## REFERENCES

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