Analysis of particle rearrangement in high-load tableting with a DEM-based elasto-plastic cohesive model

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ABSTRACT

Performance of finishing operations of pharmaceutical tablets such as coating does not only depend on process efficiency or inter-tablet variability: non-optimal process parameters as well as micro-mechanical anisotropy originated during high load compaction may facilitate chipping, edge cracking or an overall undesired breakage propensity, which can lead to the rejection of entire batches. The extent of each individual failure mechanism depends on formulation parameters (elasto-plastic mechanical properties of tablet components), compaction parameters and geometry, stress field, and impact intensity within subsequent process steps (e.g. drum coating, conveying).

Towards a better understanding of the effects of stress distribution, orientation and plastic yielding within the fabric, numerical modelling by means of continuum Drucker-Prager Cap model has been reported on numerous occasions[1]. However, due to the particulate nature of powders, densification of the powder proceeds through elasto-plastic deformation and internal particle rearrangement, which can only be captured with a partially or completely discrete approach such as Discrete Element Method (DEM). Success in this approach would lead to a better prediction of process efficiency and robustness on the basis of starting material properties.

The goal of the present study is to assess the validity of an elasto-plastic hysteretic DEM contact model, namely the so-called Edinburgh Contact Model (ECM)[2] for determining the extent of particle rearrangement. First, to yield precise and transferable methods and results, a careful calibration of loading and unloading stiffnesses (k_1 and k_2) and Coefficient of Restitution is performed with indirect micro-indentation testing for three reference materials (microcrystalline cellulose, anhydrous lactose and dicalcium phosphate dyhidrate). Second, the effect of rearrangement is studied by comparing simulations neglecting this effect with the generation of a homogeneous strain field solution with a real test case of cylindrical die compaction. The effects of long-lasting adhesion forces and friction are extracted for both scenarios.

Particle rearrangement is analysed with averaged quantities such as coordination number, average contact area, and contact orientation with fabric tensors. These magnitudes show a stronger effect of rearrangement in closed die compaction than for isostatic compaction. Finally, a good agreement with experimental data and existing statistical models for a homogeneous strain field is extracted. Results of this study help to solve the arduous and not fully understood process of modelling compaction of pharmaceutical mixtures.

REFERENCES

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