High-load compaction of pharmaceutical tablets: Model calibration approaches

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ABSTRACT

Finite Element Method (FEM) is often used to model compaction behaviour of pharmaceutical powders. However it does not provide insight how particle properties (such as: Young's modulus, coefficient of rolling/sliding friction etc.) affect bulk powder behaviour during die compaction. In this work the Discrete Element Method (DEM) is used to describe the compaction process. One of the major challenges in DEM is the definition of the particle contact model and the determination of its parameters.

The aim of this study is to compare different contact models and to develop a methodology to determine the DEM contact model parameters for compaction of pharmaceutical tablets. We consider three different contact models; Luding's, Thornton and Ning's and Morrissey's for comparison. For the DEM model calibration both single particle and bulk experiments are conducted. Nano-indentation is used to calibrate contact stiffness (loading and unloading) and AFM is used to measure pull off force between particles. On the other side bulk compression test at low (kPa) and high stress (MPa) levels is used to calibrate bulk stress-strain response during tablet compaction. The determined model parameter values are then used to simulate the tableting process at varying stress levels. Finally the simulation results are compared with experimental results. We consider three different contact models; Luding's, Thornton and Ning's and Morrissey's for comparison.