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DEVELOPMENT AND VALIDATION OF A FAST AND EFFICIENT ITERATIVE DEM CALIBRATION DATA-BASE

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Understanding tablet manufacturing processes can be challenging because of complex powder behaviour and a limited amount of data that can be collected during experimental runs. Furthermore, the cost of the materials for experimental trials can be prohibitively high, especially during the early stages of drug development. Efficient simulation tools facilitate enhanced process understanding and accelerate the process development which consequently reduces the R&D cost and risks.

For the description of granular flow, often the Discrete Element Method (DEM) method is used. The DEM accounts for each particle-particle interaction and provides a better understanding of interactions between particles on a micro-mechanical level. In our case the high-performance GPU-based code XPS is used. However, the calibration of DEM contact parameters, which is critical for accurate process simulation, takes a considerable amount of time. Therefore, an efficient calibration procedure is desirable.

In this work we report on the development of an iterative calibration procedure for contact parameters of advanced DEM model (e.g., MEPA) that leads to a data base of calibrated materials with a standardized procedure. The calibration procedure features four steps at different flow regimes and stresses including packing, compression with elastic recovery, dynamic angle of repose, and yield locus measured in a shear cell. This iterative approach is developed based on a statistical analysis of contact parameters and their influence on simulated characterization tests. This analysis also provides a statistical model that can be used for an initial estimate of the contact parameters. The calibration procedure is divided into calibration steps where each step is designed to determine a specific contact parameter. This approach ensures speed and efficiency in DEM simulation efforts.

The calibrated contact models are then benchmarked for a continuous mixing process simulation. Finally, the predicted residence time distributions are validated against the experimentally obtained step responses of the mixing equipment. A data base of calibrated materials is presented.

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