DEM simulation of the compaction behaviour of lactose powder combined with µCT analysis

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Abstract. Powder compaction is a key step in many industrial processes, where the applied mechanical stresses can cause plastic particle deformation or breakage, which influences the packing behaviour and thus the mechanical strength of the bulk material. In this work, the compaction behaviour of lactose powder is investigated experimentally and numerically to improve the predictions of compressibility and the packing structure during the compaction process. The particles are compacted under different normal stresses in an in-situ micro-computed tomography (µCT) compaction cell in a cylindrical die. The µCT imaging allows local analysis of the packing structure, particle displacements, and contact development during compaction. The experiments are used to validate simulations with the Discrete Element Method (DEM), which enables a direct comparison of the porosity and stress development in the particle bed for different particle sizes between experiment and simulation at different compaction stresses.

1. Introduction

Powder compaction is a fundamental operation in many industrial processes such as tableting, briquetting, calendaring and extrusion, where the mechanical behaviour of the particles determines the final product properties. In practice, particulate products consist of particles that are not only distributed in size but also in their mechanical properties, as commonly observed in pharmaceutical formulations. This leads to a loading situation that strongly depends on local concentration, packing arrangement, and particle properties.

During compaction, the deformation of a particle bed typically progresses through three stages: particle rearrangement, elastic deformation, and plastic deformation or even particle fracture when exceeding the mechanical material strength. In order to understand and optimize this process, continuous methods such as finite element method (FEM) or discrete methods such as the discrete element method (DEM) are commonly used.

Experimental insight into micromechanical interactions can be obtained using in-situ micro-computed tomography (µCT), which allows local analysis of the packing structure, particle displacements, and contact development during compaction.

In DEM simulations, contact forces and particle deformations can be directly resolved using suitable contact models, providing detailed insight into the micromechanical interactions that are not accessible in experiments. The elastic-plastic deformation can be described with our previous developed contact model [1] that captures the yield point at the transition from elastic to plastic deformation using measurable mechanical properties of the particles.

2. Materials and methods

The compaction behaviour of lactose powder was investigated experimentally and numerically. Lactose powder produced by spray drying was used in this study. The morphology of the lactose particles was analysed by light microscopy and scanning electron microscopy (SEM) (Figure 1).

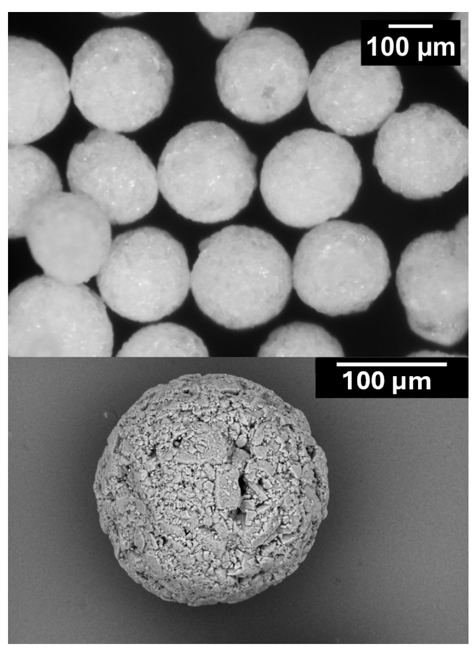

Figure 1. Optical analysis of the lactose particles with light microscope and SEM.

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The mechanical properties of the particles were conducted with single particle compression tests using a Nanoindenter (TI Premier Hysitron, Bruker). Additional compression tests were performed to investigate particle fracture behaviour under increased load.
Compaction tests were carried out with an in-situ force cell (Figure 2), which can be integrated into the µCT (TomoScope L, Werth Messtechnik GmbH). The particle bed was subjected to different normal stresses to analyse the evolution of the packing structure and the particle displacements.

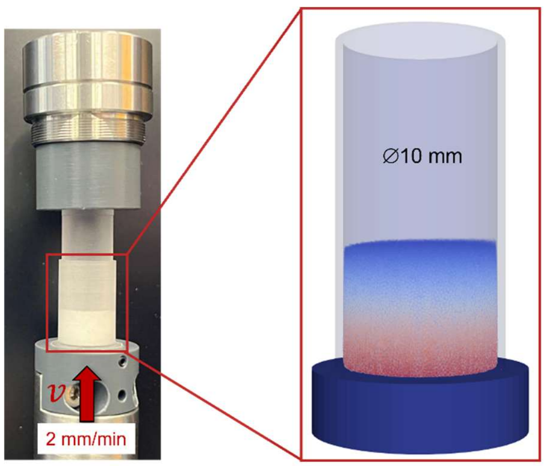

Figure 2. Experimental in-situ setup used for µCT compaction tests.

3. Results

The results from single-particle compression tests reveal that particle deformation is initially governed by elastic and plastic behaviour, followed by fracture at higher stresses (Figure 3). This indicates that particle breakage becomes relevant at elevated compaction stresses and must be considered in the analysis of the compaction process.

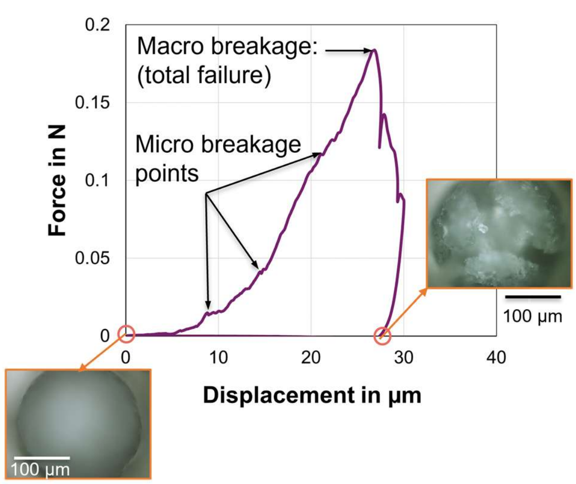

Figure 3. Typical force displacement curve of the particle compression test until breakage.

The µCT experiments provide detailed insight into the packing structure during compaction. With increasing normal stress, a densification of the particle packing is observed, accompanied by particle rearrangement, plastic deformation, and a reduction in porosity. At higher stresses, particle fracture occurs at the surface of the bed. The DEM simulations show good agreement with the experimental results in terms of porosity and overall compaction behaviour (Figure 4).

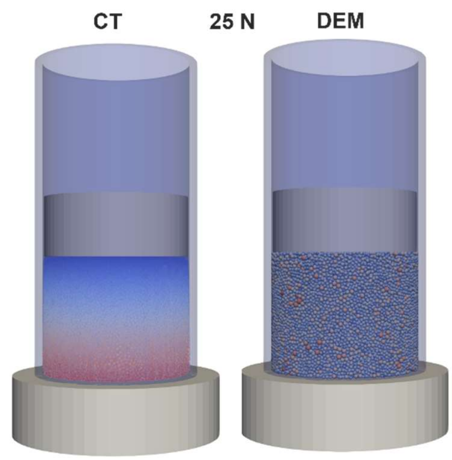

Figure 4. Compaction test at 25 N showing µCT reconstruction (left) and DEM simulation (right).

The simulations provide information on contact forces, particle deformations and stress distributions within the particle bed. An increase in contact number and local stresses is observed with increasing compaction stresses. The distribution of plastic deformation within the particle bed and the porosity distribution over the particle bed height were analysed for increasing compaction stresses. Furthermore, good agreement between experimental and numerical compressibility was observed.

4. Conclusions

This study investigated the compaction behaviour of lactose powder using a combined experimental and numerical approach based on in-situ µCT measurements and DEM simulations. The results show that compaction is governed by particle rearrangement, plastic deformation, and particle fracture at higher compaction stresses. The µCT experiments provide detailed insight into the structural evolution of the particle bed, while DEM simulations provide access to particle deformations and stress distributions. The combined approach improves the understanding of compressible particulate systems and supports the development of more predictive models for industrial compaction processes.

References

[1] Krull F., Strohner D., Antonyuk S.: Experimental methods for model parameters in the Discrete Element Method, KONA Powder and Particle Journal 43 (2026) 22-46, https://doi.org/10.14356/kona.2026006