Characterization of Mesoscopic Structure in Cohesive Powders by X-Ray Computed Tomography and Prediction by the Discrete Element Method

Andrew Abi-Mansour, Sean McClure, Michael Gentzler, and Wenjuan Zheng

Center for Materials Science and Engineering,
Merck Sharp & Dohme Corp., West Point PA 19486, USA

Understanding and predicting structural and dynamic (flow) characteristics of cohesive powder systems is a technical challenge in many powder technology processes and applications. The discrete element method (DEM) [1] is a promising approach to model the structure and flow behavior of cohesive granular systems. Advances in experimental techniques such as X-ray computed tomography (XRCT) have now enabled characterization of cohesive powder systems with sub-micron resolution. Combined with standard bulk powder characterization methods (e.g. density), this technique allows for mesoscopic structural characteristics of cohesive powder systems to be compared with DEM simulation. In this study, DEM and XRCT are used to characterize the mesoscale structure, under controlled consolidation conditions, of two cohesive 'model' (roughly spherical) powders with distinct material properties. The DEM simulations are based on a constitutive elasto-plastic model [2] that makes use of the JKR theory [3] to account for cohesive interparticle forces. Powder density and mesoscopic structure obtained from DEM simulation are compared to characterization results obtained from XRCT image analysis. The ability of DEM simulation and the contact model to accurately predict these characteristics is discussed.

References

[1] P. A. Cundall and Otto D.L. Strack. A discrete numerical model for granular assemblies. *Geotechnique*, 29(1):47–65, 1979.

[2] C. Thornton and Z. Ning. A theoretical model for the stick/bounce behaviour of adhesive, elastic-plastic spheres. *Powder technology*, 99(2):154–162, 1998.

[3] K.L. Johnson, K. Kendall, and A.D. Roberts. Surface energy and the contact of elastic solids. In *Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*, volume 324, pages 301–313. The Royal Society, 1971.