Quantifying the effect of fillers on the breakage behaviour of needle-shaped particles

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ABSTRACT

Understanding the relationship between the applied stress and the behaviour of breakable granular material is required in many chemical engineering applications. The extent of breakage depends on the properties of particles and the applied stress. In granular physics research, packings of spheres have been well studied, while considerably less attention has been given to packings of anisotropic particles or packings containing the mixture of different kinds of particles (composite packings). The presence of an additional kind of the particle inside the packing will alter packing compaction and particle breakage. The extent of such change is not well understood at the moment.

An example of a composite packing can be found in pharmaceutical tablet production. The active pharmaceutical ingredient (API), often present in the form of fragile needle-shaped crystals is mixed with other excipient (e.g. fillers) components. DEM was used to model such packing, formed from a mixture of fragile needle-shaped crystals and elastic spherical filler particles. The packing was subjected to unidirectional compression stress and the evolution of particle size distribution and other packing properties were computed for different sizes, volume fractions and elasticities of filler particles inside the packing.

We show that particle breakability in a packing is directly related to the number of contacts among particles and that it can be significantly influenced by an appropriate choice of added filler particles. The results can be used for the development of mathematical models that describe the pharmaceutical tablet production and other processes involving composite packing of fragile particles.

REFERENCES

[1] Z. Grof and F. Stepanek, "Distribution of breakage events in random packings of rodlike particles", *Phys. Rev. E*, **88**, 012205 (2013).

[2] Z. Grof, C.M. Schoellhammer, P. Rajniak and F. Stepanek, "Computational and experimental investigation of needle-shaped crystal breakage", *Int. J. Pharmaceutics*, **407**, 12-20 (2011).

[3] Z. Grof, M. Kohout and F. Stepanek, “Multi-scale simulation of needle-shaped particle breakage under uniaxial compaction”, *Chem. Eng. Sci.*, **62**, 1418-1429 (2007).