International Fine Particle Research Institute

Project Brief

Unravelling Particle Cohesion and Shape

Significant progress has been made in recent years in DEM-based simulations of granular systems. However, most models are still unable to represent faceted particles with different surface properties and surface energies between facets. While recent advances in Contact Dynamics have enabled precise DEM-like modelling of polyhedral particle contact, the role of particle shape- and facet-dependent surface properties on interactions between cohesive particles (beyond those in direct contact) have not been considered.

IFPRI wishes to fund a project to extend the Contact Dynamics approach by incorporating realistic crystalline particle shapes and surface energies and to quantitatively assess reveal how particle shape influences cohesion, local packing structure, and bulk flow properties in dry fine powders (that display macroscopic cohesive behavior arising from particle scale in the range of 0.1 – 100 um). The hoped-for outcomes of the work are development of a mechanistic understanding of shape-driven vs. surface-energy driven cohesion, identification dimensionless descriptors of shape and cohesion relevant for industrial powders, and incorporation of particle shape into DEM models used in industry.

The objectives of this project are:

- Develop a DEM-based framework using the Contact Dynamics method incorporating:
    - polyhedral particle shapes
    - facet-dependent surface energies
    - interparticle cohesion and friction
- Simulate bulk properties for a variety of realistic, *faceted* crystal shapes to tease apart the roles of particle shape and interparticle cohesion on bulk powder properties such as packing density and cohesivity
- Validate the new models via comparison with experimentally measured powder properties (e.g. experimental tapped densities, porosity, tensile strength, stiffness) for a range of habits, sizes, and polymorphic forms of one or more model systems.

The choice of model systems is unrestricted, as long as the particles are faceted and the surface energies of the facets are known or can be measured or computationally predicted with confidence (as for metals or simple ceramics). Spherical particles, polymeric systems, gels, and glass beads are out of scope.