Technische Universität Braunschweig

iPAT Institut für Partikeltechnik

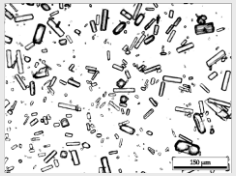
in cooperation with:

KIT Karlsruher Institut für Technologie

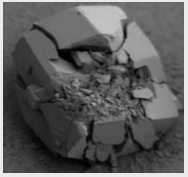
VM

Master thesis: Simulation of crystal fractures in a filter cake

The selective crystallisation of proteins as a combined processing and formulation step represents a possible alternative to a cost- and resource-intensive chromatography step in downstream processing. Besides the challenge of selectively crystallising the protein in the desired shape and size, another important aspect is the mechanical stability of the crystals. Compared to conventional crystals, these are much more sensitive and can break even at low pressures. Even filtration pressures of a few bar lead to breakage for some crystal systems, which makes the downstream solid-liquid separation much more difficult. Therefore, the fracture behaviour of crystals in a cluster (filter cake) is of particular interest. The fracture behaviour of single crystals has already been characterised on rod-shaped lysozyme crystals using a nanoindenter. The aim is now to simulate the fracture behaviour in a cluster using the Discrete Element Method (DEM) on the basis of these characteristic values in combination with crystal size distributions of real rod-shaped lysozyme crystals.



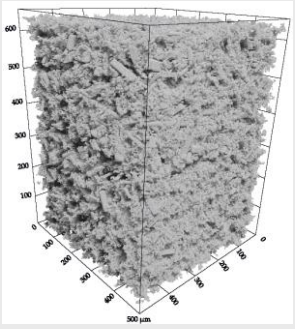
Crystal



Crystal breakage

The focus is on the following tasks:

- Implementation of the fracture behaviour of protein crystals in the discrete element method (DEM) software Rocky.
- Setup of the simulation environment: particle bed with correct size distribution, particle shape and porosity
- Compression of the filter cake between two planes by means of external loading
- Evaluation of the simulations with regard to the fracture of crystals



µCT-scan of a filter cake structure

We can arrange a personal meeting at any time to discuss this, or other topics, without obligation.

Start: **By arrangement**

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