

## 2 Bachelor-Projects - Chemical Engineering (Verfahrenstechnik) Modeling of Cohesive Particulate Matter on the Computer

Cohesive particulate matter is of central importance for chemical engineering, as well as a plurality of other sciences, e.g., space or earth sciences that are interested in the mechanical properties of particulate systems. While a variety of particle-scale models for cohesive systems are available (e.g., models for van der Waals forces), the effect of model details on bulk properties (e.g., the yield locus, or the bulk density) are not well explored. Also, most available force models were built for infinitely stiff particles. This image of infinitely stiff particles conflicts with the assumption of Discrete Element Method (DEM)-based simulators that rely on (often very) soft particles.

One Bachelor project should review recent progress in the field of force models (with a focus on van der Waals and electrostatic forces) for modelling cohesive particular matter. Based on an existing implementation into the simulator LIGGGHTS®, simulations should be performed that probe the effect of model details on predictions for macroscopic cohesive properties of powders. Specifically, stiffness correction well approaches, as as models for rough surfaces should be investigated in detail.



Image of a comet recorded during the "Rosetta" mission. Especially under micro-gravity conditions cohesive forces are relevant, necessitating a precise calibration of model parameters, and careful model selection (http://www.esa.int/Our\_Activities/Space\_Science/Rosetta).

Another bachelor thesis should focus on a thorough dimensional analysis of the flow and fluidization of cohesive (polydisperse) powders, considering conditions on earth and under micro-gravity conditions (e.g., as present on a comet). Also, this thesis should explore a relevant parameter space with DEM simulation using LIGGGHTS<sup>®</sup>.

The prospective students must be able to communicate in English, and should have a solid background in Matlab and/or C/C++. Of course, strong interest in particulate systems is required.

We offer

- high industrial and scientific relevance (e.g., for powder processing, petroleum engineering, or space science)
- computer(s) with installed, fully documented, and tested DEM simulation software LIGGGHTS®. Tutorials, screencasts, and personal training on the DEM simulator can be provided. Based on the interest of the student(s), an introduction to C/C++ programming can be provided to allow students to extend the simulation software
- desk and office space for writing the bachelor thesis

## Contact

Stefan Radl, <u>radl@tugraz.at</u>; 0680 / 12 22 168 The bachelor thesis projects can be started earliest by April 1<sup>st</sup> 2017. However, thesis work during the summer months would be preferred.