Development and implementation of coupling between the DEM and PBM simulation frameworks

Nowadays, computer modelling plays an important role in the deployment of new processes, as well as in the investigation and optimization of existing ones. Generally, the currently available methods for modelling of solids processes can be distinguished according to the time and length scales on which they are applied. On the macroscopic scale, semi-empirical population balance models (PBM) can be effectively used to describe a time-dependent change of a particle collective. One of the main advantages of the PBM is the relative small computational load, which allows describing industrial scale apparatuses and performing dynamic simulation over long time intervals. However, the PBM is based on empirical parameters for description of the process kinetics. Such PBM parameters as aggregation rate, breakage function, etc. in most cases are obtained empirically for a specific parameter space and cannot be effectively used outside of it.

Alternatively, there exist microscale calculation methods, such as the discrete element method (DEM), which allows describing all occurring micro processes with very high detail. With DEM, each individual particle is treated as a separate object, which allows to consider material properties of each single granule properly, as well as to describe cohesive forces caused due to the presence of liquid bridges. However, one of the main drawbacks of this method is a high computational load and a very limited number of particles that can be modelled simultaneously. Therefore, direct simulation of industrial or even lab-scale apparatuses is, in most cases, impossible.

Another novel type of method which can be applied for modelling of the problems described above is a multiscale simulation strategy. It can be effectively used to perform physically-based detailed simulation of industrial scale apparatuses. The main idea of such approach is to combine models of different time and length scales into one multiscale framework. Using microscale calculations that are performed over a short time interval or where only a small region of apparatus is modelled, the parameters for a macroscopic model can be approximated. Afterwards, the macroscopic model is used to simulate a real apparatus over a large time interval.

In this project, a directly coupled DEM-PBM simulation framework will be developed. For this purpose, the already available DEM simulation framework MUSEN and the system for dynamic simulation of interconnected solids processes Dyssol will be used. Standardization of interfaces and their implementation will play a central role in this project.

Working plan:

1. Literature review about the PBM and DEM.
2. Development of the DEM-PBM coupling interface.
3. Implementation of the DEM-PBM coupling subsystem.
4. Verification and performance tests using the MUSEN and Dyssol software.
5. Writing the report.