

Fully Coupled Multiphase Simulation of a bottom-spray Wurster Coater using a hybrid CPU/GPU CFD/DEM Approach

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ABSTRACT

Where most of the DEM simulations focus on dry material handling, some highly important applications involve liquid chemical sprays. Here, granular material is functionalized by chemical means in order to vitalize surfactant reactions or to realize coating on tablets. Effects like dissolution and wet agglomeration or partial sticking of wet particles need to be modelled in tandem with the force driven particle interactions. Moreover, in coupled simulations different physical effects like heat transfer and mass transfer between liquid phase and solid phase need to be considered properly. Chemical engineering processes are often lasts for several minutes to hours to finish up. The simulation of such processes is a challenge as well as the huge amount of particles.

Using an in-house DEM code, we simulate a lab-scale Wurster coater. The Wurster coater is a bottom spray granulator with a draft tube inside the bed. The tube creates a circulating flow pattern. Air streams into the granulator through a plate at the bottom, which consists of regions with different porosities. The plate has larger orifices below the Wurster tube and therefore the fluidization gas enters at higher velocity below the tube. Whilst processing, air induces a circulation regime of the particles through the Wurster tube. Liquid suspension is sprayed continuously by a bottom spray nozzle. The particles grow according to their residence time in the spray zone. Additionally the sprayed liquid causes agglomeration.

We use the commercial AVL Fire® solver for the fluid phase and our in-house GPU DEM code XPS for the modelling of the solid phase. Due to the spraying particles get polydisperse and agglomerate. The spray nozzle is modelled by a ray threading technique, which simulates a conical wet fog. The particles are able to wear a film of variable thickness and their mass varies along with the film coating.

Efficient simulations of coupled multiphase flow in the million particle range can be achieved by using hybrid CPU/GPU computing on a desktop workstation. The optimization of a coating process demonstrates the strength of tailored simulation tools for chemical and pharmaceutical engineering. The advantage of our CFD-DEM hybrid CPU/GPU simulation method is, that the codes run inside a single workstation but on separate computing platforms. We are able, to do simulations for up to 25 million particles.

REFERENCES

- [1] JAJCEVIC D., SIEGMANN E., RADEKE C. and KHINAST J. G., (2013), "Large-scale CFD-DEM simulations of fluidized granular systems", *Chemical Engineering Science*, Vol 98, pp 298-310, July 2013.