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A multiscale perspective on crystal growth and dissolution

Many pharmaceutical formulations employ active pharmaceutical ingredients (APIs) in crystalline form. The growth behavior of the different facets of a crystal affects the morphology and consequently the further processing e.g. in filtration, drying or tableting steps. In the final product formulation the dissolution behavior is of paramount importance for the bioavailability of the drug. There is not only the thermodynamics in terms of the solubility which is important but also the dynamics, i.e. the dissolution rate in a certain environment. A fundamental understanding of crystal growth and dissolution leading to a predictive modeling and simulation thereof would aid product and process design alike. Although being fundamentally governed by the molecular interactions such molecular scale of investigation alone does not provide feasible concepts for process simulation at an actual batch crystallization scale. For the predictive simulation of crystal growth or dissolution a multiscale simulation approach is needed, in which molecular-level behavior is used to parametrize methods capable of simulating up to the microscale and beyond, where the theoretical results would be industrially relevant and easily comparable to experimental results. By spanning the range from Molecular Dynamics (MD) simulation via Monte-Carlo (MC) simulations and continuum based transport models towards Population Balance Models (PBM) such multiscale strategy is presented. For exemplary test cases this strategy has already proven to be successful. Key elements of the transition between the different scales and the experimental validation will be presented.

Biography

Heiko Briesen holds the Chair for Process Systems Engineering at Technical University of Munich (TUM). He studied Chemical Engineering in Karlsruhe at the currently named Karlsruhe Institute of Technology (KIT) and the University of Cincinnati. During his academic career at RWTH Aachen, the Max-Planck-Institute in Magdeburg and Technical University of Munich (TUM) he worked on several aspects of modeling, simulation and mathematical optimization for different applications spanning petrochemical, bio engineering, food and pharmaceutical processes. One of the focal applications for many years is the formulation of crystals. To achieve predictive modeling tools for crystal formulations a wide range of tools on various scales from molecular dynamics, via Monte-Carlo-simulations and population balance models, to final process flow sheeting are employed.

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