

A numerical method for the simulation of uni- and bivariate population balance systems

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Crystallization processes are fundamental operations in obtaining particulate products in the chemical industry. Such processes can be modeled by a *population balance system* describing different mechanical phenomena, e.g. nucleation, growth, aggregation, breakage and transport of particles. This system consists of the incompressible Navier–Stokes equations for describing the flow field in the domain $\Omega \subset \mathbb{R}^3$ and scalar convection-diffusion equations which model the energy balance (temperature) and the concentration of dissolved species. Coupled to these equations, there is an equation for the particle size distribution.

Altogether, a population balance system contains equations which are defined in domains with different dimensions. In fact, the flow field, the concentrations of dissolved species and temperature are defined in a three-dimensional spatial domain, while the PSD depends also on the *internal* coordinates, which describe additional properties of the particles (e.g. *diameter*, *volume*) resulting in uni-variate models. More geometrical properties of the particles are often needed to characterize the particles for crystallization processes. Thus, extensions to the multivariate models yield more trustful models of such processes, improving the accuracy of simulations.

In particular, **uni-variate** and **bi-variate** population balance models are based on one- and two-dimensional geometrical characterization of the individual particles (*diameter*, *volume*, or *main axis in case of anisotropic particles*), resulting in four-dimensional (4D) and five-dimensional (5D) PSD systems.

The talk presents an approach for the simulations of the population balance systems (e.g. the synthesis of urea for the uni-variate model, the production of potassium dihydrogen phosphate for the bi-variate model). This approach is based on implicit time-stepping schemes, finite element, and finite difference discretizations.

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