Numerical Simulation of a Calcium Carbonate Precipitation

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The precipitation of barium sulphate is modeled by a population balance system describing

- an incompressible flow field (Navier–Stokes equations),
- an isothermal chemical reaction (nonlinear convection–diffusion–reaction equation),
- a population balance equation for the particle size distribution (linear transport equation).

The solution of each individual equation possesses its difficulties:

- in applications, the flow is often turbulent,
- it is important that one obtains oscillation–free solutions for the concentrations in the chemical reaction,
- the particle size distribution depends not only on time and space but also on one or even more properties of the particles (interior coordinates); that means, one has to solve an equation in $\mathbb{R}^d$, $d \geq 4$ in applications.

It turns out that the simulation of population balance systems is rather challenging.

We will present first steps in the simulation of the precipitation of barium sulphate. The flow and the chemical reaction will be considered in a two–dimensional domain. The particle size distribution possesses one interior coordinate (the diameter of the particles). For the particles, nucleation and growth are modeled. Topics included into the talk are the discretization of the individual equations and numerical simulations for different physical and chemical parameters.

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