Model reduction methods for microemulsion-assisted particle precipitation

B. Niemann[1], A. Voigt[2], K. Sundmacher[1,2]

[1]Physical and Chemical Process Engineering (PCP)
[2]Otto-von-Guericke University Magdeburg, Process Systems Engineering

POPULATION BALANCE SYSTEMS

Motivation

- Identification of the particle formation mechanism on molecular scale including particle nucleation, particle growth and droplet exchange
- Investigation of the complex redistribution behavior of reactant ions
- Analysis of the influence of hydrodynamics on the particle formation

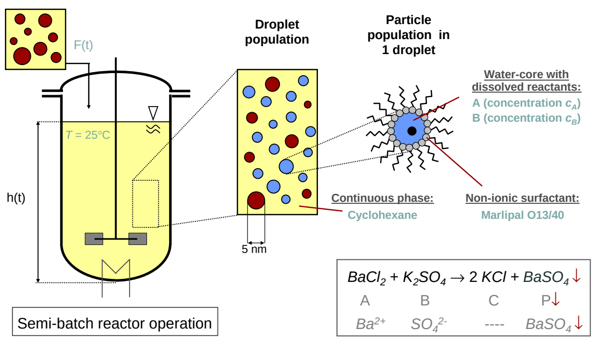


Figure 1: Process scheme, reaction system and phase structure.

Approach

- Combined experimental and model-based process analysis:
  - Experimental identification of control parameters for a tailored particle design and analysis of the particle formation dynamics

    ⇒ *Rigorous TEM analysis of the particle size distribution dynamics*
  - Derivation of a Population Balance Model framework including models on different levels of complexity for diverse applications

    ⇒ *Definition of reasonable physically and chemically motivated assumptions and determination of a detailed reference model*

    ⇒ *Development of a reliable model reduction concept*

    ⇒ *Implementation of appropriate microkinetic rate law approaches based on experimental findings*

    ⇒ *Parameter estimation of unknown kinetic parameters*

Experimental Results [1]

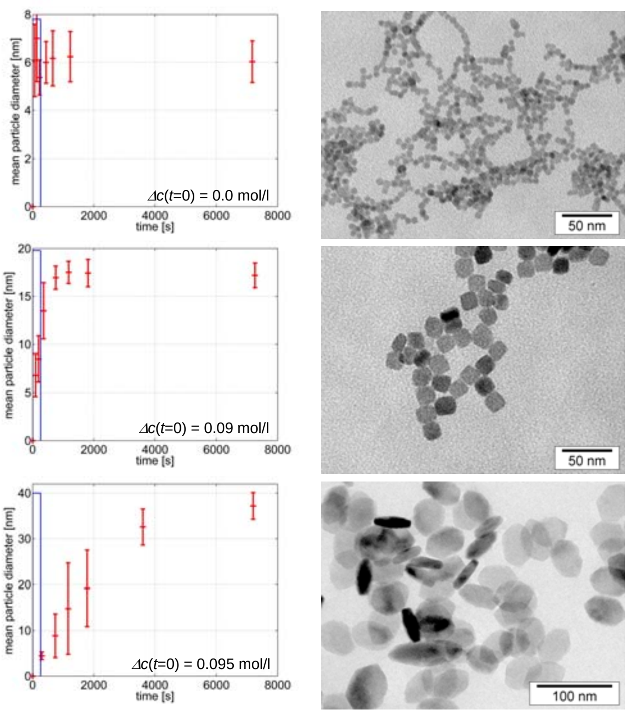


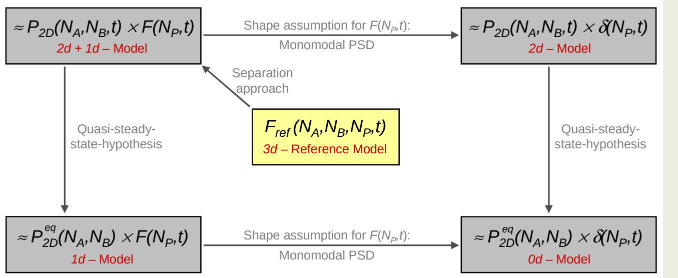
Figure 2: Dynamics of the mean particle diameter with standard deviation (left; feeding period in blue; initial concentration difference between reactor and feed: $\Delta c(t{=}0)$); corresponding TEM pictures of $BaSO_4$ nanoparticles in final state (right).

Modeling & Simulation Results

Assumptions:

1. The reactor is ideally macro-mixed
2. The water content of particle-free droplets and droplets with particles below the barrier size is monodisperse (equal water volume)
3. At maximum there exists only one particle per droplet
4. No agglomeration or breakage of particles

Model Reduction [2]:



2d + 1d - Model:

Reactant probability distribution with discrete internal coordinates:

$$\frac{dP_{2D}(N_A,N_B,t)}{dt} = \underbrace{p_{ex}^{\pm}(N_A,N_A',N_A'',N_B,N_B',N_B'',t)}_{\text{droplet exchange}} + \underbrace{p_{feed}^{+}(N_A,N_B,t)}_{\text{feed}} + \underbrace{p_{nuc}^{\pm}(N_A,N_B,t)}_{\text{nucleation}} + \underbrace{p_{gro}^{\pm}(N_A,N_B,N_P,t)}_{\text{growth}}$$

Balance for particle-free droplets:

$$\frac{dF(0,t)}{dt} = f_{nuc}^{-}(N_A,N_B,t) + f_{feed}^{+}(N_A,N_B,t)$$

Balance for the droplet number distribution with particles:

$$\frac{dF(N_P,t)}{dt} = f_{nuc}^{+}(N_A,N_B,t) + f_{gro}^{\pm}(N_A,N_B,N_P,t)$$

Droplet exchange term:

$$p_{ex}^{\pm}(N_A,N_A',N_A'',N_B,N_B',N_B'',t) = 2\cdot k_{ex}\cdot\frac{N_M(t)}{N_{M,0}}$$

$$\times\left(\sum_{N_A'=0}^{N_{I,max}}\sum_{N_B'=0}^{N_{I,max}}\sum_{N_A''=0}^{N_{I,max}}\sum_{N_B''=0}^{N_{I,max}}\beta(N_A,N_A',N_A'',N_B,N_B',N_B'')\cdot P_{2D}(N_A',N_B',t)\cdot P_{2D}(N_A'',N_B'',t)\right.$$

$$\left.-P_{2D}(N_A,N_B,t)\cdot\sum_{N_A'=0}^{N_{I,max}}\sum_{N_B'=0}^{N_{I,max}}P_{2D}(N_A',N_B',t)\right)$$

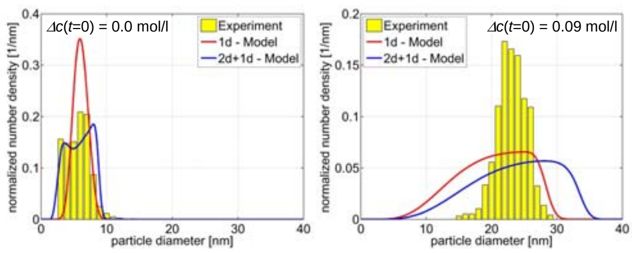


Figure 3: Comparison of experimental and simulation results [3].

Collaborations

- Prof. Ramkrishna, Purdue University, West Lafayette, USA
- Prof. Thévenin, Otto-von-Guericke University, Magdeburg
- Dr. Veit, Otto-von-Guericke University, Magdeburg

Publications

[1] B. Niemann, P. Veit & K. Sundmacher (2008), 'Nanoparticle precipitation in reverse microemulsions: Particle formation dynamics and tailoring of particle size distributions', Langmuir 24(8), 4320-4328

[2] Niemann, B. & Sundmacher, K. (2008), 'Reduced discrete population balance model for precipitation of barium sulfate nanoparticles in nonionic microemulsions', Chemical Engineering Journal, http://dx.doi.org/10.1016/j.cej.2008.06.012

[3] Niemann, B. & Sundmacher, K. (2007), 'Two coupled population balances with three discrete internal coordinates for nanoparticle precipitation in colloidal systems', in '3rd International Conference on Population Balance Modelling (PBM2007)', Québec, Canada

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