411a A Comparison of Deterministic Population Balance Equations and Stochastic Monte-Carlo Approaches for Modelling the Particle Precipitation in Microemulsions

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The nanoparticle production using microemulsions is a very interesting alternative to gas phase methods or to bulk phase precipitation reactions. The nanodroplets in microemulsions can be used as small reactors in a precipitation reaction. They are filled with different reactants and the coalescence-redispersion phenomena between the droplets lead to a controlled uniform mixing, followed by chemical reaction, nucleation and growth. The slow-down of fast phenomena due to the coalescence is very important to enable the control of particle sizes and particle size distributions.

For a proper process analysis and control a large variety of parameters and process conditions have to be investigated. A suitable modeling and simulation will help to find via sensitivity analysis the most suitable control parameters of the process. Population balance modeling of microemulsion precipitation has shown good potential for simulating the particle size distributions although the underlying droplet coalescence and redispersion phenomena makes this a high dimensional problem which is hard to tackle by the common PBE approaches [1]. As an alternative Monte-Carlo simulation are applicable for this type of problem [2,3]. Here the multidimensionality of the process model can be incorporated more easily. The disadvantages lie in the increase of computation time when the considered system sizes are extended to cover all underlying phenomena appropriately with good statistics.

In this presentation a thorough comparison of the advantages and disadvantages of PBE modeling and Monte-Carlo simulation will be shown on several sensitivity studies as for example on feed rate conditions, droplet sizes and initial reactant concentrations. The data of both approaches, particle sizes and particle size distributions, will be compared with respect to computational efficiency and accuracy. Also a detailed comparison to experimental data of barium sulfate nanoparticle production in a technical microemulsion precipitation process will show how both model approaches can be used for different problems of technical importance. In an optimization cycle several different parameters like nucleation and growth rate of the underlying models have to be adjusted and properly compared.

The main goal of the work will consist in finding arguments for different possible modeling strategies on two important aspects, the model validation and the application of model simulations for control purposes. This will help in establishing the microemulsion precipitation as a viable alternative for the large-scale production of tailor-made nanoparticles.

[1] B. Niemann, D. Adityawarman and K. Sundmacher: Multidimensional population balance modeling of barium sulfate precipitation in microemulsions, AIChE 2004 Annual Meeting Conference Proceedings (2004).

[2] D. Adityawarman, A. Voigt, P. Veit and K. Sundmacher: Precipitation of BaSO4 Nanoparticles in a Non-ionic Microemulsion: Identification of Suitable Control Parameters, Chemical Engineering Science 60, p.3371-3383 (2005).

[3] A. Voigt, D. Adityawarman and K. Sundmacher: Size and distribution prediction for nanoparticles produced by microemulsion precipitation: A Monte-Carlo simulation study, Nanotechnology 16, S429-S434 (2005).