

Multidimensional property design of crystal populations using a systems approach

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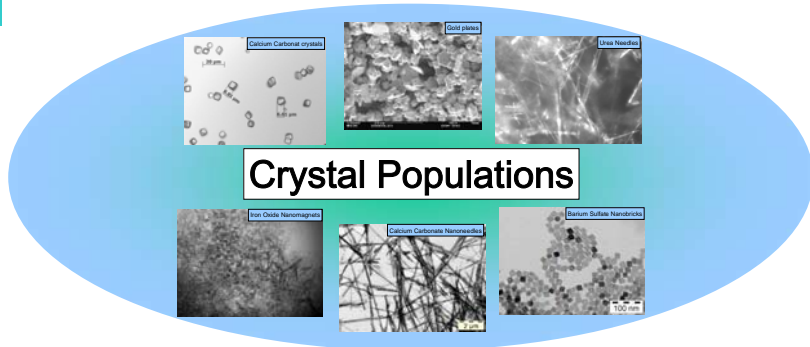
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Material → Process → Product

Crystal Properties

- Size
- Shape
- Composition
- Morphology
- Hardness
- Surface Structure



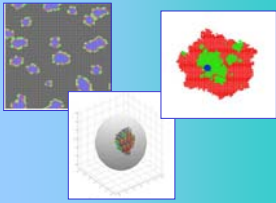
Applications

- Surface coatings
- Ceramic materials
 - Catalyst
- Pharmaceuticals
- Semiconductors
- Magnetic liquids

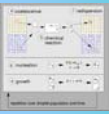
Systems approach combining theory and experiments

Theory

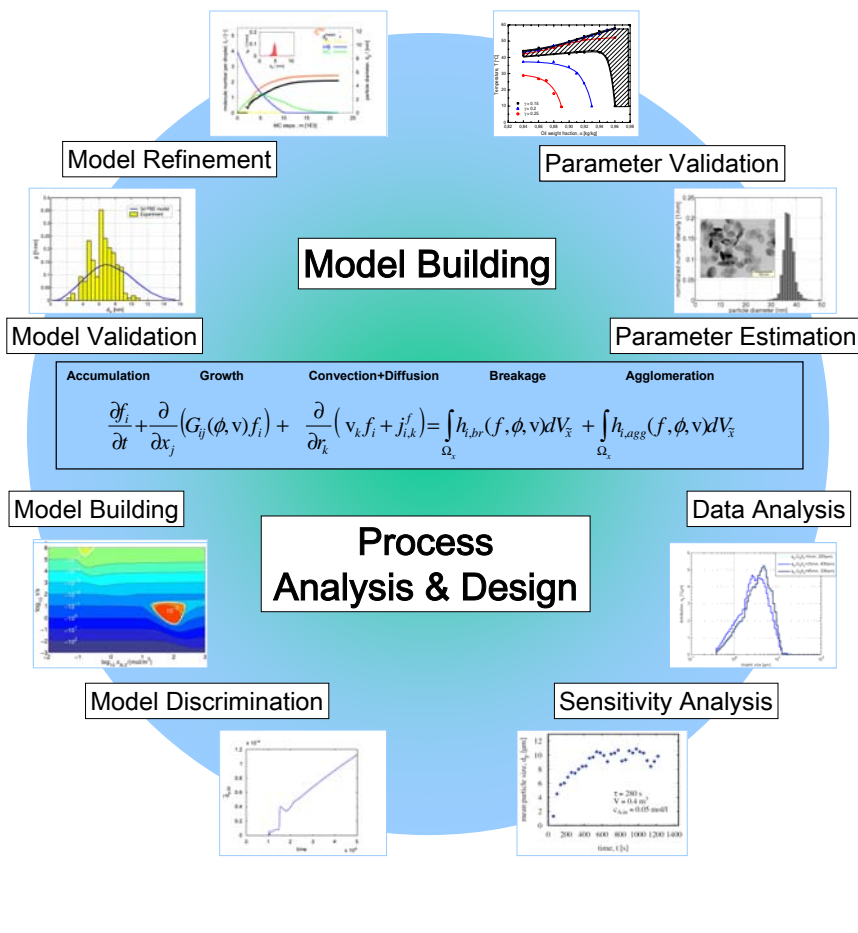
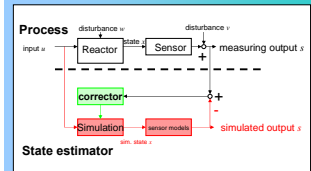
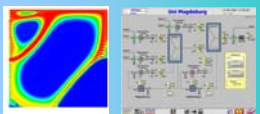
• Molecular Simulation



• Mesoscale simulation

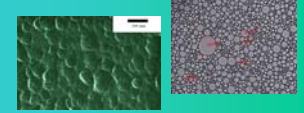


• Process Level Simulation



Experiment

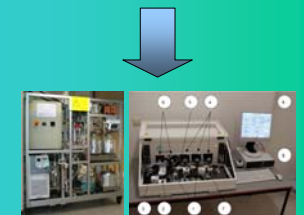
• Micro/Mini-Emulsion droplets



• Flask



• Reactor



• Miniplant/Microplant

Application requirements → Process Analysis & Design → Product Properties

Publications

[1] Voigt, A., Adityawarman D. and Sundmacher, K. Size and distribution prediction for nanoparticles produced by microemulsion precipitation: A Monte-Carlo Simulation study, *Nanotechnology* **16** (2005) S429-434.
 [2] Adityawarman, D., Voigt, A., Veit, P. and Sundmacher, K. Precipitation of BaSO₄ nanoparticles in a non-ionic microemulsion: Identification of suitable control parameters, *Chemical Engineering Science* **60** (2005) 3373-3383.
 [4] Rauscher, F., Veit, P. and Sundmacher, K. Analysis of a technical-grade w/o microemulsion and its application for the precipitation of calcium carbonate nanoparticles, *Colloid Surf. A-Physicochem. Eng. Asp.* **254** (2005) 183-191.
 [5] Niemann, B., Rauscher, F., Adityawarman, D., Voigt, A. and Sundmacher, K. Microemulsion-assisted Precipitation of Particles: Experimental and Model-based Process Analysis, *Chemical Engineering and Processing* **45** (2006) 917-935.
 [6] Heineken, W., Flockerzi, D., Steyer, C., Voigt, A. and Sundmacher, K. Nonlinear dynamics of continuous precipitation reactors: A model based analysis, *Chemical Engineering Science* **62** (2007) 4896-4902.
 [7] Voigt, A. and Sundmacher, K. Herstellung maßgeschneiderter Nanopartikel durch Fällung in Mikroemulsionen, *Chemie Ingenieur Technik* **79**(3) (2007) 229-232.
 [8] John, V., Mitkova, T., Roland, M., Sundmacher, K., Tobiska, L. and Voigt, A. Simulations of population balance systems with one internal coordinate using finite element methods, *Chemical Engineering Science* (2008) in press.
 [9] Mangold, M., Boeck, A., Schenkendorf, R., Steyer, C., Voigt, A. and Sundmacher, K. Two State Estimators for the Barium Sulfate Precipitation in a Semi-Batch Reactor, *Chemical Engineering Science* (2008) in press
 [10] Borchert, C., Nere, N., Ramkrishna, D., Voigt, A. and Sundmacher, K. On the prediction of crystal shape distributions in a steady-state continuous crystallizer, *Chemical Engineering Science* (2008) in press.
 [11] Gao, Y., Voigt, A., Hilfert, L. and Sundmacher, K. Nanodroplet Cluster Formation in Ionic Liquid Microemulsions *ChemPhysChem* **9**(11), 1603-1609 (2008).

