109 Modeling and Synthesis of agglomeration and disintegration process of oxide nanoparticles for solving population balance equations

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ABSTRACT

Agglomeration and disintegration of oxide nanoscaled particles is a challenge to be met when controlling particle size distributions in many areas like precipitation, crystallization and milling. The presented work shows a combined experimental as well as numerical approach to determine particle size distribution using titanium dioxide as the model substance. Modeling must now include the influence of colloidal surface forces and hydrodynamic forces on particle aggregation and breakup. The superposition of the population balance models for agglomeration and grinding with the appropriate kernels leads to a system of partial differential equations, which can be solved in various ways numerically. Here a modified h-p Galerkin algorithm which is implemented in the commercially available software package PARSIVAL developed by CiT (CiT GmbH, Rastede, Germany). This includes a comparison of the derived particle size distributions, moments and its accuracy depending on the starting particle size distribution and the used agglomeration and breakage kernels. Finally, the computational effort of both methods in comparison to the prior mentioned parameters is evaluated in terms of practical application.

Keywords: Population balance model, Nanoparticle, Titanium dioxide, Precipitation