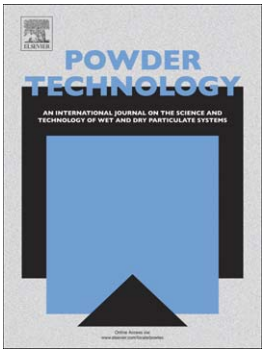

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Modelling zirconia nanoparticles prepared by supercritical water hydrothermal synthesis using population balance equation

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Abstract

In this study, based on the population balance equation, a numerical simulation model was developed to predict particle size distribution (PSD) of zirconia in a supercritical water hydrothermal synthesis (SWHS) process. Using the method of moment, the corresponding equation was solved to obtain particle number density and PSD. Precipitation process (including nucleation and growth with/without aggregation) was simulated using this model in a batch reactor. Results indicated good convergence of experimental PSDs and those predicted considering aggregation, confirming the significance of taking this phenomenon into account in PSD modeling which was validated subsequently. Furthermore, effects of precursor concentration and pH on evolution of supersaturation, precipitation kinetics and PSD of zirconia nanoparticles were also investigated. Results revealed that increased concentration and decreased pH led to higher supersaturation, faster reaction rate, and more zirconia particles formation with larger sizes.

Keywords: zirconia nanoparticles, particle size distribution, nucleation/growth rate, supercritical water.