Poster SCF5

CFD Simulation in Supercritical Water: Design of a Reactor and Prediction Tool for Morphology of ZnO Nanoparticles

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Direct information about fluids under supercritical water conditions is complicated due to the engineering restrictions (such as corrosion and mechanical constraints). Numerical investigations based on Computational Fluid Dynamics (CFD) calculations are widely used in order to get extensive information on the fluid behavior, particularly to help the design of process. This study presents the numerical investigations performed on a supercritical water reactor. CFD calculations allowed to design and optimize the presented reactor. Thus, this reactor satisfies the following criteria: (i) instantaneous mixing of fluid flows, to aid in the formation of many small metal oxide nuclei which is desirable for nanoparticle formation; (ii) short residence time combined with a narrow residence time distribution, to minimize the subsequent particle growth and to obtain narrow particle size distribution; (iii) minimal heating of the aqueous metal salt stream prior to the inlet in the reactor, followed by an immediate and rapid heating of the salt solution within the reactor, to prevent undesirable precipitation/deposition of metal salts in the inner pipes and (iv) strong net downstream flow/eddies for the rapid transport of product particles out of the reactor, to prevent particle accumulation within the reactor and to minimize subsequent particle growth. This reactor was tested with numerous nanopowders in order to verify that a homogeneous particle size distribution has been obtained (and thus a weak influence of vortices). The reliability of the process has also been tested on long time experiments in order to verify that no plugging has occurred.
Continuous hydrothermal flow synthesis process has shown great advantages concerning the control of particle size and morphology through optimization of processing parameters command. In this study, a CFD model is suggested for ZnO nanoparticles morphology prediction using a population balance approach.The effects of basis concentration and hydrodynamics are investigated. Results show that the CFD approach is a valuable predictive tool for controlling the size and the shape of nanoparticles from SCW parameters. However, some additional knowledge on nucleation, crystal growth and aggregation mechanisms are useful in order to get a better agreement.