Poster MS3

The Nucleation and Growth of Zinc Oxide Nanoparticles from Ambient to Supercritical Conditions

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Supercritical Water (SCW) Synthesis is an eco-friendly process for the production of metal oxid nanoparticles. Some applications require a perfect control of particle characteristics such as size, shape and distribution. The use of surfactants helps to control these parameters. However, those chemicals may have an impact on powder behavior as well as on the environment. Thus, the need to develop a green, safer and direct synthesis of metal oxide is essential. In supercritical domain, water dielectric constant and density decrease leads to a modification of the solubility of inorganic compounds such as metal oxides. Thus, a higher supersaturation rate is achieved allowing to a faster nucleation kinetic and, then the formation of nanoparticles. To better control the particle distribution of powder in SCW conditions, a rapid and homogeneous heating of the solution has to be performed during the synthesis. Also a short residence time is necessary to obtain nanoparticles. In this prospect, our team has developed a continuous hydrothermal production process of nano-oxides in sub- and supercritical conditions since 2001. Many metal oxides can be prepared as simple oxides (ZnO, TiO_2 . . .) and polycationic oxides (Ce_x Zr_{1-x} O_2 . . .).

Nevertheless, only few studies introduce mechanisms of metal oxide nanoparticles formation i SCW conditions. In this study, ZnO is used as a model material to understand the metal oxide nanoparticles synthesis, especially in supercritical conditions. To investigate ZnO nucleation and growth phenomena according to synthesis parameters (T, P . . .), the evolution of particle morphology and size was observed by TEM. Crystallite sizes were determined by means of X-Ray diffraction line broadening analysis. Assuming a cylindrical shape of ZnO crystallites based on the hexagonal crystal structure, the length and diameter were determined by XRD pattern decomposition method and compared to TEM observations. Moreover, a Computational Fluid Dynamics (CFD) model was developed; chemical reactions can be extracted from this model. Hence, the particle size characteristics have been determined using a population balance model and compared to experimental results. Based on such results, several mechanisms are suggested such as a zinc oxide nanoparticle growth mechanism according to the pressure and the temperature.