

Fluid-Particle Dynamics of Nanoparticle Synthesis in Flame Spray Reactors

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Introduction

Flame spray pyrolysis (FSP; Mädler et al., 2002) has been shown a versatile and economic process for nanoparticle production (Wegner et al., 2011). It relies on inexpensive metal-containing liquid precursors, which are atomized by a dispersion gas and ignited to form a spray flame. Following spray droplet evaporation and precursor conversion nanoparticles grow by nucleation, coagulation, sintering and/or surface growth. Fundamental understanding of the complex interactions between these mechanisms is required for transfer of the current laboratory batch process to continuous manufacturing scale (Gröhn et al., 2012).

The objective of this work is the development of a computational fluid-particle dynamics model covering all important process steps to assist reactor operation, optimization and scale-up. The model is performance-tested and validated for the example of zirconia (ZrO_2) nanoparticle production.

Method

Spray, fluid, combustion and aerosol dynamics are integrated in a computational fluid dynamics (CFD) solver to predict product zirconia nanoparticle properties without adjustable parameters or need of experimental input data. By assuming immediate particle formation on precursor oxidation and a self-preserving particle size distribution a robust and computationally feasible description of the process could be constructed (Gröhn et al., 2011). In order to obtain insight into the FSP process for scale-up the model is extended to include both laboratory- and pilot-scale reactor geometries.

Fourier-transform infrared spectroscopy, Phase-doppler anemometry and nanoparticle sampling in-situ the flame are employed for characterizing the temperature, velocity and particle growth profiles of the flame reactor and are used for validation of the computational code (Gröhn et al., 2012).

Results and Discussion

Figure 1 shows simulated primary particle diameters compared with the measurements for 3, 5 and 7 l/min dispersion O_2 and 4 ml/min 0.5 M Zr precursor flow. The predicted primary particle size is strongly influenced by the description of zirconia sintering as revealed by comparing three literature expressions for the solid-state diffusion coefficient, showing that an adequate description of sintering is required for the development of accurate aerosol synthesis models.

Parametric simulations with the CFD model revealed that nanoparticle production rate can be increased without affecting the primary particle size by

maintaining constant precursor to dispersion gas flow. Successful scale-up using such method was demonstrated with experiments.

A simple and robust model describing flame spray synthesis of zirconia nanoparticles has been developed that does not rely on experimental input data and is well suited for process design, reactor optimization and scale-up of the widely-used FSP process for synthesis of a broad spectrum of nanostructured materials.

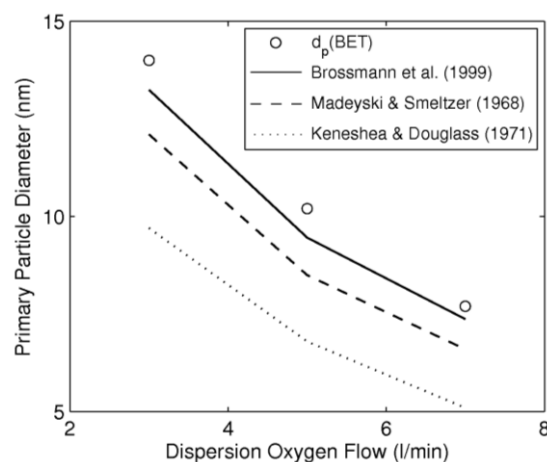


Figure 1. Effect of sintering rate on the predicted primary particle diameters for 4 ml/min of 0.5 M Zr precursor. Grain boundary diffusivity of Brossmann et al. (1999) gave best agreement with experiments.

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