Simulation of the flow field in a nanoparticle synthesis spray flame reactor including a particle coating process

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Nanoparticles are widely used in consumer products, industrial applications and in the energy industry.

For the aerosol synthesis of nanoparticles, spray flame reactors are commonly used which enable high production rates of particles with different properties and structures. A liquid precursor-solution is injected into the reactor, atomized, evaporated and ignited, forming a self-sustaining spray flame. The nanoparticles are formed inside the flame through nucleation and condensation and increase due to growth, agglomeration and aggregation. Further downstream, the core-shell structured particles are coated continuously by injection of a secondary precursor (Teleki et al., 2008).

The efficiency of the particle production and the quality of the products depend on the thermodynamic state, the precursor and the particle residence time in the different zones of the reactor (Kammler et al., 2001, Teleki et al., 2009). The control and optimization of the synthesis process therefore requires knowledge of these parameters, which can be obtained from computational fluid dynamics (CFD). Figure 1 shows an example of the temperature distribution inside a spray flame reactor calculated with CFD and the stages of the process.

In this work, CFD simulations were used to investigate variations of process parameters and reactor geometry in order to find the best operating conditions. The investigated reactor (Hardt et al., 2011) is applied for synthesis of Silica (SiO_2) coated Titania (TiO_2) particles from Titanium-tetraisopropoxide (TTIP).

The calculations were performed in two stages: in the first stage, the spray flame was simulated in order to determine the shape and the quantity of the heat source in direct vicinity of the burner. The spray was modelled with an Euler-Lagrangian approach using a two-way coupling of flow and droplets considering the evaporation process. The turbulence was modelled using the k-epsilon closure and the combustion using the Eddy Dissipation approach.

For the second stage, the complete reactor including the coating nozzle was calculated using a simplified heat release model. This simplification enabled the simulation of a large number of geometry variants at acceptable cost. The dispersed particle phase was described using an Eulerian approach and the particle dynamics were modelled with a method of moments using a locally monodisperse particle size distribution (Kruis et al., 1993). The quality of the mixing in the coating zone was determined from the ratio of particle number concentration and secondary precursor concentration. This is a simplified estimate that does not consider the joint PDF of particle and precursor concentration. The transport equations for the dispersed phase and the population balance model were implemented in the framework of the open source CFD software OpenFOAM.
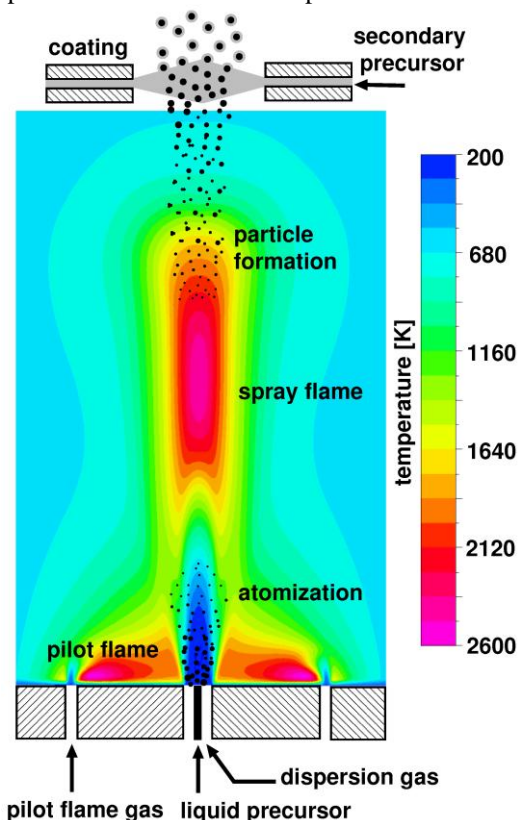

Figure 1: Temperature distribution and illustration of the particle production process inside a spray flame reactor.

Teleki, A., M.C. Heine, F. Krumeich, M.K. Akhtar, and S.E. Pratsinis (2008), *Langmuir*, 24, 12553-12558.

Kammler, H. K., L. Mädler, S. E. Pratsinis (2001), *Chemie Ingenieur Technik*, 73, 6, 708.

Teleki A., B. Buesser, M.C. Heine, F. Krumeich, M.K. Akhtar, S.E. Pratsinis (2009), *Industrial & Engineering Chemistry Research*, 48, 1, 85-92.

Hardt, S., A. Hamid, C. Weise, I. Wlokas, H. Wiggers and C. Schulz (2011), *Experimental and Numerical Investigation of Flame Spray assisted TiO2 Synthesis from Titaniumtetraisopropoxide,* 5th European Combustion Meeting, Cardiff.

Kruis, F.E., K.A. Kusters, S.E. Pratsinis (1993), *Aerosol Science and Technology*, 19, 4, 514-526.