LES modeling of nano particles synthesis in the SpraySyn burner

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Abstract

We present Large Eddy Simulations of the turbulent combustion and subsequent nano particle formation in the SpraySyn burner (DFG Priority Program SPP 1980). The SpraySyn burner was designed for gas phase material synthesis at reproducible operation conditions and was optimised such that simulation can focus on the spray combustion and aerosol dynamics. These goals were achieved by a setup with three concentric streams: in the center, the liquid and a dispersion gas form a spray, this is surrounded by a premixed pilot flame and an inert coflow outside. The pilot and the coflow streams pass a sinter matrix, that ensures homogeneous flow conditions around the central spray nozzle and a thick, easy to resolve mixing layer between the streams.
The inhouse LES code PsiPhi is applied to characterize the combustion regimes and the conditions experienced by the synthesized nano particles. Subgrid turbulence is described by Nicoud's Sigma model, the spray droplets are described by a Lagrangian approach with momentum and mass transfer with the Eulerian phase. Combustion is described by precalculated tables, following the Premixed Flamelet Generated Manifold (PFGM) approach. The tables are acessed with two mixture fractions (for pilot flame products and ethanol) and a progress variable. The nano-particle dynamics are modeled either by a i) computationally costly, polydisperse sectional model, which accounts for nucleation and growth by coagulation, or ii) a monodisperse model which accounts for nucleation, coagulation and sintering. The models resolve the particle size distribution in time and space, but do not consider their subgrid distribution and its effect on aggregation. The presentation will show where the more costly sectional modelling is required and where the simpler model will suffice, and a parameter is derived to identify the respective regions.

Keywords: Spray, Nano, Combustion

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