High-fidelity simulations of spray formation in flame spray pyrolysis

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Abstract

Flame spray pyrolysis (FSP) is a promising approach for production of nanoparticles with tailored functionalities. Those functionalities are determined by the particle properties (e.g. size, morphology, homogeneity, configuration, and/or crystallite properties), which mainly are controlled by the temperature, concentration distribution inside the reactor, and the residence time of particles in certain regions. It was shown that the spray characteristics influence the particle formation, which may be used to tailor particle properties. However, this requires a comprehensive knowledge of the impact of spray formation on the particle formation. In order to overcome the lack of knowledge, a detailed and accurate characterization of the spray formation is necessary.

In this work, the spray formation of a standardized burner for researching FSP (SpraySyn burner), which is based on the coaxial atomization principle, is studied using high-fidelity simulations in order to understand the influence of the dispersion gas flow on the spray characteristics. One-way coupled simulations of the turbulent nozzle internal flow of the dispersion gas and primary breakup are used. Coupling is achieved by imposing the unsteady velocity field of the nozzle outlet plane as inlet conditions for the interface resolving primary breakup simulations. The nozzle internal flow is computed in a large-eddy simulation (LES) using the compressible, structured, high-order finite-difference solver of the in-house code CIAO, which solves the fully compressible Navier-Stokes equations using an explicit time-integration scheme. Primary breakup is computed as direct numerical simulation (DNS) with a 2ndorder coupled 3D unsplit Volume of Fluid/level-set method, which employs a hybrid Lagrangian/Eulerian discretization of the convective terms and a ghost fluid method consistent pressure projection.

Simulations of the complex SpraySyn nozzle geometry and a fully developed turbulent pipe with SpraySyn nozzle outlet geometry are performed. The simulation framework is validated with experimental data of the SpraySyn geometry and the simulated spray characteristics of both nozzle geometries are discussed with respect to relevant nozzle internal flow quantities.

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