198f Large-Scale Simulation of Nanoparticle Synthesis in Turbulent Reacting Flows. the Effects of Turbulence and Mixing on Formation and Growth

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Vapor-phase synthesis of nano-structured materials is a cost-effective and controllable means for the production of wide variety of materials, including those used in fuel cells, energetic materials, and chemical sensors, amongst others. In nearly all high-rate synthesis methods for nanoparticles, chemical precursors are brought together by turbulent mixing to form particle nuclei that grow rapidly due to surface addition and aggregation. Next-generation applications of nanoparticles will require precise control of product quality when synthesis methods are scaled up. Predicting nanoparticle aggregation starting with detailed knowledge chemical and thermodynamic histories, as well as the time-dependent flow properties are key to the reliable scale-up of high-rate synthesis methods. This work describes a computational approach which provides knowledge of particle field in a model free manner, as a function of space, time, and size. We show the effects of mixing on nanoparticle area during flame synthesis, the segregation of nanoparticles in turbulent jets, and the effects of turbulence on the growth of nanoparticles.