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Supercritical Water Flow Influence on Synthesizing Uniformly Sized Nanoparticles ELIZABETH RASMUSSEN, University of Washington-Seattle, Argonne National Laboratory, R. JACKSON SPURLING, University of Tennessee- Knoxville, Argonne National Laboratory, MAI K. TRAN, Rice University, Argonne National Laboratory, JIE LI, Argonne National Laboratory, ARGONNE NATIONAL LABORATORY COLLABORATION — The drastic thermodynamic changes of supercritical phase fluids near the critical point leads to a highly tunable environment for nanoparticle synthesis. Once synthesis conditions are defined, a high throughput method that results in uniformly sized nanoparticles is necessary for the successful transition of new materials into the real-world. Understanding the flow characteristics of such complex reactors aids in optimized operation, hence this work describes how these characteristics inside a built reactor affect the temperature field, which can lead to variation in particle size and distribution. High-fidelity 3D numerical simulations provide insight using the Helmholtz energy-based Span-Wagner equation of state for a reactor operated at 23-24 MPa and 650-700K (very close to water's critical point of 647K and 22.1MPa). From simulations and experimental validation, it is concluded that a quenching flow is not necessarily the optimal method to achieving a uniform, low-temperature field and furthermore, partial quenching can decrease uniformity while having a negligible effect on mean particle size. By comparing different operating conditions, the properties of supercritical fluids as a suitable reaction medium for uniformly sized nanoparticles is discussed.

Elizabeth Rasmussen
University of Washington, Argonne National Laboratory

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