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Mesoscale Modelling of Nano-Particle Growth Under Flow ROHAN VERNEKAR, TIMM KRÜGER, School of Engineering, Institute for Multiscale Thermofluids, University of Edinburgh —

Nanoparticles have wide potential for future applications, from drug delivery to surface coatings. Control over (e.g. silica) nanoparticle morphology, size, porosity and dispersity is crucial for realisation of their use[1]. The physics of growth of such particles under flow conditions is not well understood, thus making their industrial scale-up challenging.

We present a mesoscale lattice Boltzmann (LB) algorithm that models growth of nanoparticles under particle resolved flow conditions *via* chemical species deposition. The method combines fluid LB for hydrodynamics, advection-diffusion LB for species transport with resolved Newtonian nanoparticle dynamics and a novel mesoscale adsorption boundary condition for growth[2]. The algorithm is benchmarked for various 2D cases and provides excellent results. Our method enables the study of flow effects on growth, morphology and size distribution of nanoparticle suspensions, and advances nanoscale particle synthesis modelling.

[1]Hyde, E. D. E. R. et al. Colloidal Silica Particle Synthesis and Future Industrial Manufacturing Pathways: A Review. Ind. Eng. Chem. Res. 55, 88918913 (2016).
[2]Krüger, T. et al. The Lattice Boltzmann Method: Principles and Practice. (Springer International Publishing, 2017).

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